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Bis{3,5-di-*tert*-butyl-*N*-[(4-dimethylamino)phenyl]-salicylaldiminato}cobalt(II)

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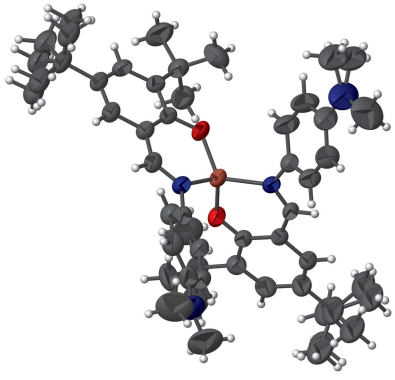
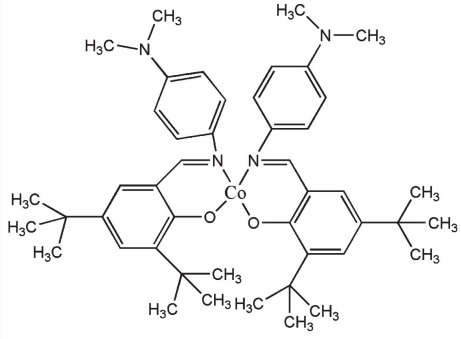
Structural data: full structural data are available from iucrdata.iucr.org

In the title complex [systematic name: bis(2,4-di-*tert*-butyl-6-{*N*-[4-(dimethylamino)phenyl]carboximidoyl}phenolato)cobalt(II)], $[Co(C_{23}H_{31}N_2O)_2]$, the cobalt(II) atom is coordinated by pairs of O and N atoms in a distorted tetrahedral coordination geometry. The dihedral angles formed by the aromatic rings of the same ligand are 51.99 (11) and 36.58 (9)°. The molecular conformation features weak intramolecular C—H···O hydrogen bonds. In the crystal, inversion-related pairs of complex molecules are linked into dimers by weak C—H···π interactions. The methyl C atoms of *tert*-butyl groups have rotational disorder, with site occupancies of 0.647 (7) and 0.617 (6) for the major components and 0.353 (7) and 0.383 (6) for the minor components. One of the methyl C atoms of the dimethylamino groups is also disordered over two orientations, with an occupancy ratio of 0.75 (4):0.25 (4).

3D view



Chemical scheme



Structure description

Metal complexes of N- and O-chelating ligands have attracted considerable attention because of their interesting physicochemical properties and pronounced biological activities. The N and O atoms play a key role in the coordination of metals at the active sites of numerous metallobimolecules (Nair *et al.*, 2006). Schiff base–cobalt(II) metal complexes are constantly used in numerous applications varying from catalysis to pharmaceuticals (Holla *et al.*, 2003). We herein report the synthesis and the structure of the title compound (Fig. 1). The metal cation has a distorted tetrahedral coordination geometry provided by two O and two N atoms. The Co—O distances [Co1—O1 = 1.8844 (19), Co1—O2 = 1.8882 (19), Co1—N1 = 1.980 (2), Co1—N2 = 1.984 (2) Å] agree well with the values observed in related structures (Adam *et al.*, 1997; Chen *et al.*, 2014, 2015).

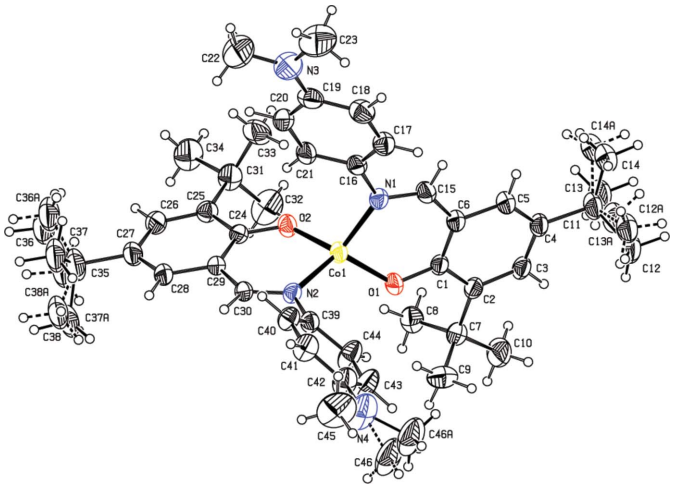


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

The dihedral angle between the aromatic rings C1–C6 and C24–C29 is 85.85 (15)° while the C16–C21 ring makes a dihedral angle of 55.59 (17)° with the C39–C44 ring. The molecular conformation is stabilized by weak C—H···O hydrogen bonds (Table 1). The crystal structure exhibits dimeric units formed by weak C—H···π interactions (Table 1) occurring between inversion-related complex molecules..

Synthesis and crystallization

Methanolic solutions of the Schiff base (1 mmol, 10 ml) and $Co(AcO)_2{\cdot}H_2O$ (0.5 mmol; 10 ml) were mixed thoroughly and boiled under reflux for 4–6 h, and then cooled to room temperature. The resulting precipitate was filtered, washed in ice-cold ethanol and dried *in vacuo*. X-ray quality single crystals were grown by layering a $CHCl_3$ (3 ml) solution of the compound with CH_3CN (5 ml).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The methyl C atoms of the *tert*-butyl groups exhibit rotational disorder, with site occupancies of 0.647 (7) (C12–C14) and 0.617 (6) (C36–C38) for the major components. One methyl C atom of the dimethylamino groups is disordered over two orientations with site occupancies of 0.75 (4) and 0.25 (4) for the major (C46*A*) and minor (C46) components, respectively. The anisotropic displacement parameters of the disordered C atoms were restrained by SIMU instructions within 0.001 standard deviations. DELU restraints were also applied. The C—C and C—N bond lengths involving the disordered atoms were restrained to 1.50 (1) and 1.40 (1) Å, respectively. A potential solvent-accessible void of 179 Å^3 was detected but no residual electron density could be located in the final difference-Fourier map.

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

Cg is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*C*···O1	0.96	2.38	3.007 (4)	123
C9—H9*A*···O1	0.96	2.28	2.953 (4)	126
C32—H32*C*···O2	0.96	2.33	2.974 (4)	124
C33—H33*C*···O2	0.96	2.28	2.925 (4)	124
C45—H45*B*···*Cg*^{i}	0.96	2.96	3.914 (5)	171

Symmetry code: (i) $-x, -y, -z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_{23}H_{31}N_2O)_2]$
M_r	761.92
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	295
a, *b*, *c* (Å)	11.5598 (3), 13.3787 (4), 17.3035 (5)
α, β, γ (°)	111.756 (1), 96.694 (2), 98.293 (1)
V (Å^3)	2417.01 (12)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.39
Crystal size (mm)	0.34 × 0.30 × 0.26
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.691, 0.905
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41823, 9288, 6088
R_{int}	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.058, 0.175, 1.07
No. of reflections	9288
No. of parameters	567
No. of restraints	100
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.73, −0.42

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2016/4* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

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References

Adam, K. R., Anderson, P. A., Astley, T., Atkinson, I. M., Charnock, J. M., Garner, C. D., Gulbis, J. M., Hambley, T. W., Hitchman, M. A., Keene, F. R. & Tiekink, E. R. T. (1997). *J. Chem. Soc. Dalton Trans.* pp. 519–530.
Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, Y. M., Gao, Q., Chen, W. Q., Gao, D. D., Li, Y. H., Liu, W. & Li, W. (2015). *Chem. Asian J.* **10**, 411–421.
Chen, Y. M., Gao, Q., Zhang, H. F., Gao, D. D., Li, Y. H., Liu, W. & Li, W. (2014). *Polyhedron*, **71**, 91–98.
Holla, B. S., Veerendra, B., Shivananda, M. K. & Poojary, B. (2003). *Eur. J. Med. Chem.* **38**, 759–767.

Nair, B., Shah, A., Baluja, S. & Chanda, S. (2006). *J. Serb. Chem. Soc.* **71**, 733–744.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* A**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

full crystallographic data

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Crystal data

$[Co(C_{23}H_{31}N_2O)_2]$
M_r = 761.92
Triclinic, $P\overline{1}$
a = 11.5598 (3) Å
b = 13.3787 (4) Å
c = 17.3035 (5) Å
α = 111.756 (1)°
β = 96.694 (2)°
γ = 98.293 (1)°
V = 2417.01 (12) Å^3
Z = 2
$F(000)$ = 818
D_x = 1.047 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5165 reflections
θ = 2.4–22.4°
μ = 0.39 mm^{-1}
T = 295 K
Block, colourless
0.34 × 0.30 × 0.26 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.691, T_{max} = 0.905
41823 measured reflections
9288 independent reflections
6088 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 26.1°, θ_{min} = 2.0°
h = −14→14
k = −16→16
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.175
S = 1.07
9288 reflections
567 parameters
100 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0983P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.2392 (3)	0.3564 (2)	0.32262 (16)	0.0487 (6)	
C2	0.3243 (3)	0.3202 (2)	0.36672 (17)	0.0521 (7)	
C3	0.2911 (3)	0.2850 (2)	0.42796 (18)	0.0572 (8)	
H3	0.346893	0.259851	0.455435	0.069*	
C4	0.1792 (3)	0.2847 (2)	0.45161 (18)	0.0569 (8)	
C5	0.1001 (3)	0.3215 (2)	0.41019 (18)	0.0588 (8)	
H5	0.025030	0.322522	0.424485	0.071*	
C6	0.1260 (3)	0.3586 (2)	0.34614 (18)	0.0545 (7)	
C7	0.4508 (3)	0.3225 (3)	0.3475 (2)	0.0630 (8)	
C8	0.5119 (3)	0.4395 (3)	0.3655 (2)	0.0771 (10)	
H8A	0.591067	0.440021	0.353756	0.116*	
H8B	0.515485	0.485217	0.423896	0.116*	
H8C	0.467668	0.467191	0.330149	0.116*	
C9	0.4461 (4)	0.2495 (3)	0.2558 (3)	0.0921 (12)	
H9A	0.395195	0.271678	0.219923	0.138*	
H9B	0.415340	0.174508	0.246384	0.138*	
H9C	0.524698	0.256007	0.242988	0.138*	
C10	0.5286 (4)	0.2817 (4)	0.4031 (3)	0.1014 (14)	
H10A	0.493158	0.207711	0.393612	0.152*	
H10B	0.534843	0.328325	0.461670	0.152*	
H10C	0.606484	0.283637	0.388876	0.152*	
C11	0.1529 (3)	0.2444 (3)	0.5206 (2)	0.0769 (8)	
C12	0.1685 (9)	0.1236 (5)	0.4929 (4)	0.0885 (12)	0.647 (7)
H12A	0.117868	0.079598	0.439116	0.133*	0.647 (7)
H12B	0.147390	0.095968	0.534309	0.133*	0.647 (7)
H12C	0.249872	0.120355	0.487947	0.133*	0.647 (7)
C13	0.2446 (7)	0.3136 (6)	0.6022 (4)	0.0916 (15)	0.647 (7)
H13A	0.322956	0.303763	0.592126	0.137*	0.647 (7)
H13B	0.227103	0.290383	0.646548	0.137*	0.647 (7)
H13C	0.241023	0.389810	0.618742	0.137*	0.647 (7)
C14	0.0284 (6)	0.2520 (7)	0.5411 (5)	0.0919 (13)	0.647 (7)
H14A	0.014724	0.324414	0.550798	0.138*	0.647 (7)
H14B	0.022157	0.237374	0.590866	0.138*	0.647 (7)
H14C	−0.029876	0.198886	0.494298	0.138*	0.647 (7)
C12A	0.0924 (15)	0.1241 (7)	0.4790 (7)	0.0908 (14)	0.353 (7)
H12D	0.092668	0.092999	0.520950	0.136*	0.353 (7)
H12E	0.134447	0.085520	0.436326	0.136*	0.353 (7)
H12F	0.011852	0.117418	0.453513	0.136*	0.353 (7)
C13A	0.2612 (10)	0.2610 (12)	0.5856 (8)	0.0911 (15)	0.353 (7)
H13D	0.237021	0.264323	0.637544	0.137*	0.353 (7)
H13E	0.314318	0.328509	0.595521	0.137*	0.353 (7)
H13F	0.301098	0.200811	0.564899	0.137*	0.353 (7)
C14A	0.0690 (12)	0.3134 (12)	0.5702 (8)	0.0904 (16)	0.353 (7)
H14D	−0.006326	0.297730	0.533796	0.136*	0.353 (7)
H14E	0.103741	0.390146	0.589833	0.136*	0.353 (7)

H14F	0.057614	0.295111	0.617851	0.136*	0.353 (7)
C15	0.0334 (3)	0.3962 (2)	0.31094 (18)	0.0563 (7)	
H15	−0.037059	0.390362	0.331465	0.068*	
C16	−0.0729 (3)	0.4689 (2)	0.22694 (17)	0.0524 (7)	
C17	−0.1871 (3)	0.4126 (3)	0.2210 (2)	0.0637 (8)	
H17	−0.195965	0.350816	0.234135	0.076*	
C18	−0.2850 (3)	0.4452 (3)	0.1967 (2)	0.0727 (9)	
H18	−0.359553	0.406323	0.194602	0.087*	
C19	−0.2774 (3)	0.5363 (3)	0.1743 (2)	0.0705 (9)	
C20	−0.1621 (3)	0.5927 (3)	0.1802 (2)	0.0687 (9)	
H20	−0.152657	0.654627	0.167303	0.082*	
C21	−0.0632 (3)	0.5580 (3)	0.20448 (18)	0.0594 (8)	
H21	0.011820	0.595416	0.205829	0.071*	
C22	−0.3705 (5)	0.6594 (5)	0.1289 (4)	0.151 (2)	
H22A	−0.327061	0.723158	0.176810	0.226*	
H22B	−0.449454	0.669574	0.114471	0.226*	
H22C	−0.330701	0.648895	0.081687	0.226*	
C23	−0.4932 (4)	0.5161 (5)	0.1508 (4)	0.151 (2)	
H23A	−0.494799	0.439769	0.138368	0.227*	
H23B	−0.550859	0.522928	0.109300	0.227*	
H23C	−0.511786	0.550584	0.206005	0.227*	
C24	0.2719 (2)	0.6722 (2)	0.20125 (16)	0.0455 (6)	
C25	0.3247 (3)	0.7857 (2)	0.24113 (18)	0.0551 (7)	
C26	0.3539 (3)	0.8404 (3)	0.1900 (2)	0.0693 (9)	
H26	0.389296	0.914604	0.216468	0.083*	
C27	0.3342 (4)	0.7929 (3)	0.1020 (2)	0.0741 (10)	
C28	0.2816 (3)	0.6844 (2)	0.06418 (19)	0.0621 (8)	
H28	0.266534	0.650532	0.005385	0.075*	
C29	0.2488 (2)	0.6212 (2)	0.11110 (16)	0.0458 (6)	
C30	0.1986 (2)	0.5076 (2)	0.06280 (16)	0.0463 (6)	
H30	0.184593	0.485998	0.004329	0.056*	
C31	0.3491 (3)	0.8427 (3)	0.3376 (2)	0.0731 (10)	
C32	0.4384 (4)	0.7915 (4)	0.3751 (3)	0.1115 (16)	
H32A	0.448902	0.823535	0.435723	0.167*	
H32B	0.513290	0.805160	0.358142	0.167*	
H32C	0.409178	0.713704	0.354919	0.167*	
C33	0.2319 (4)	0.8322 (3)	0.3708 (2)	0.0974 (13)	
H33A	0.177258	0.865466	0.347069	0.146*	
H33B	0.247505	0.868635	0.431381	0.146*	
H33C	0.197880	0.755883	0.354564	0.146*	
C34	0.4014 (4)	0.9676 (3)	0.3675 (3)	0.1069 (15)	
H34A	0.345418	1.001360	0.345413	0.160*	
H34B	0.474303	0.977415	0.347251	0.160*	
H34C	0.416611	1.001249	0.428225	0.160*	
C35	0.3697 (5)	0.8590 (3)	0.0497 (3)	0.1238 (15)	
C36	0.3825 (11)	0.9787 (5)	0.0901 (6)	0.1324 (18)	0.617 (6)
H36A	0.457761	1.010161	0.128056	0.199*	0.617 (6)
H36B	0.319442	0.995862	0.121122	0.199*	0.617 (6)

H36C	0.378756	1.008537	0.047385	0.199*	0.617 (6)
C37	0.2571 (8)	0.8347 (6)	−0.0220 (5)	0.1301 (17)	0.617 (6)
H37A	0.190961	0.856860	0.004003	0.195*	0.617 (6)
H37B	0.237030	0.757545	−0.056947	0.195*	0.617 (6)
H37C	0.275610	0.875241	−0.056114	0.195*	0.617 (6)
C38	0.4587 (9)	0.8060 (7)	−0.0010 (6)	0.1289 (17)	0.617 (6)
H38A	0.471838	0.837219	−0.041844	0.193*	0.617 (6)
H38B	0.428227	0.728322	−0.029810	0.193*	0.617 (6)
H38C	0.532436	0.818811	0.036344	0.193*	0.617 (6)
C36A	0.3089 (15)	0.9562 (10)	0.0745 (10)	0.1322 (18)	0.383 (6)
H36D	0.333634	1.002369	0.045685	0.198*	0.383 (6)
H36E	0.330181	0.997481	0.134535	0.198*	0.383 (6)
H36F	0.224215	0.930419	0.058881	0.198*	0.383 (6)
C37A	0.3976 (17)	0.8000 (11)	−0.0333 (7)	0.1303 (19)	0.383 (6)
H37D	0.434525	0.851823	−0.053821	0.195*	0.383 (6)
H37E	0.325697	0.756405	−0.072038	0.195*	0.383 (6)
H37F	0.451032	0.752984	−0.028568	0.195*	0.383 (6)
C38A	0.4954 (10)	0.9361 (10)	0.1014 (7)	0.1305 (18)	0.383 (6)
H38D	0.553657	0.891584	0.100900	0.196*	0.383 (6)
H38E	0.488368	0.977080	0.158805	0.196*	0.383 (6)
H38F	0.519715	0.986066	0.075569	0.196*	0.383 (6)
C39	0.1211 (3)	0.3227 (2)	0.02700 (17)	0.0513 (7)	
C40	0.0333 (3)	0.3022 (3)	−0.04044 (19)	0.0605 (8)	
H40	0.002898	0.360479	−0.045698	0.073*	
C41	−0.0110 (3)	0.1980 (3)	−0.1005 (2)	0.0742 (9)	
H41	−0.071273	0.186971	−0.145150	0.089*	
C42	0.0327 (4)	0.1093 (3)	−0.0957 (2)	0.0823 (11)	
C43	0.1216 (4)	0.1305 (3)	−0.0271 (3)	0.1016 (15)	
H43	0.153801	0.072747	−0.022423	0.122*	
C44	0.1630 (4)	0.2342 (3)	0.0339 (2)	0.0834 (11)	
H44	0.219977	0.245209	0.080453	0.100*	
C45	−0.0965 (6)	−0.0143 (4)	−0.2300 (3)	0.143 (2)	
H45A	−0.167146	0.009784	−0.212692	0.215*	
H45B	−0.116122	−0.091118	−0.266179	0.215*	
H45C	−0.063260	0.026790	−0.260142	0.215*	
C46	0.063 (4)	−0.075 (3)	−0.164 (3)	0.152 (6)	0.25 (4)
H46A	0.136583	−0.050238	−0.177732	0.228*	0.25 (4)
H46B	0.023307	−0.144706	−0.208211	0.228*	0.25 (4)
H46C	0.078034	−0.084242	−0.111487	0.228*	0.25 (4)
C46A	0.010 (2)	−0.0919 (8)	−0.1400 (9)	0.155 (6)	0.75 (4)
H46D	0.089134	−0.101603	−0.146220	0.233*	0.75 (4)
H46E	−0.046122	−0.156089	−0.179465	0.233*	0.75 (4)
H46F	−0.000541	−0.081030	−0.083336	0.233*	0.75 (4)
N1	0.0330 (2)	0.43793 (18)	0.25358 (14)	0.0506 (6)	
N2	0.1700 (2)	0.43048 (17)	0.08950 (13)	0.0465 (5)	
N3	−0.3767 (3)	0.5688 (4)	0.1488 (2)	0.1057 (12)	
N4	−0.0112 (4)	0.0029 (3)	−0.1565 (2)	0.1211 (14)	
O1	0.26661 (18)	0.38732 (17)	0.26223 (12)	0.0586 (5)	

O2	0.24583 (18)	0.61680 (15)	0.24693 (11)	0.0555 (5)
CO1	0.18236 (3)	0.46551 (3)	0.21245 (2)	0.04969 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0650 (14)	0.0425 (15)	0.0427 (14)	0.0144 (13)	0.0106 (12)	0.0201 (12)
C2	0.068 (2)	0.0421 (15)	0.0498 (16)	0.0136 (13)	0.0111 (14)	0.0206 (13)
C3	0.074 (2)	0.0530 (18)	0.0533 (17)	0.0214 (15)	0.0070 (15)	0.0296 (14)
C4	0.078 (2)	0.0535 (17)	0.0477 (16)	0.0153 (15)	0.0127 (15)	0.0278 (14)
C5	0.071 (2)	0.0628 (19)	0.0530 (17)	0.0158 (16)	0.0174 (15)	0.0315 (15)
C6	0.0666 (16)	0.0554 (17)	0.0505 (16)	0.0163 (14)	0.0141 (12)	0.0287 (13)
C7	0.071 (2)	0.066 (2)	0.0652 (19)	0.0236 (16)	0.0148 (16)	0.0361 (16)
C8	0.083 (2)	0.074 (2)	0.077 (2)	0.0095 (19)	0.0156 (19)	0.0350 (19)
C9	0.097 (3)	0.082 (3)	0.090 (3)	0.034 (2)	0.031 (2)	0.015 (2)
C10	0.091 (3)	0.135 (4)	0.125 (4)	0.051 (3)	0.031 (3)	0.090 (3)
C11	0.111 (2)	0.0800 (19)	0.0583 (17)	0.0217 (18)	0.0234 (15)	0.0449 (16)
C12	0.126 (3)	0.085 (2)	0.076 (2)	0.027 (2)	0.022 (2)	0.053 (2)
C13	0.127 (3)	0.096 (3)	0.064 (2)	0.026 (3)	0.015 (2)	0.045 (2)
C14	0.118 (3)	0.100 (3)	0.080 (3)	0.025 (3)	0.035 (2)	0.054 (2)
C12A	0.123 (3)	0.093 (3)	0.079 (2)	0.024 (3)	0.029 (2)	0.054 (2)
C13A	0.128 (3)	0.092 (3)	0.071 (2)	0.027 (3)	0.016 (2)	0.050 (2)
C14A	0.118 (3)	0.099 (4)	0.078 (3)	0.029 (3)	0.038 (3)	0.053 (3)
C15	0.0612 (16)	0.0652 (19)	0.0501 (16)	0.0156 (14)	0.0145 (13)	0.0291 (14)
C16	0.060 (2)	0.0617 (18)	0.0428 (14)	0.0209 (15)	0.0140 (13)	0.0245 (13)
C17	0.065 (2)	0.067 (2)	0.0631 (19)	0.0134 (17)	0.0117 (16)	0.0302 (16)
C18	0.061 (2)	0.095 (3)	0.068 (2)	0.0235 (19)	0.0130 (17)	0.035 (2)
C19	0.066 (2)	0.105 (3)	0.0531 (18)	0.042 (2)	0.0182 (16)	0.0343 (19)
C20	0.090 (3)	0.079 (2)	0.0600 (19)	0.040 (2)	0.0245 (17)	0.0408 (17)
C21	0.063 (2)	0.073 (2)	0.0563 (17)	0.0219 (16)	0.0161 (15)	0.0372 (16)
C22	0.128 (5)	0.204 (6)	0.199 (6)	0.102 (4)	0.050 (4)	0.137 (5)
C23	0.079 (4)	0.197 (6)	0.216 (7)	0.071 (4)	0.035 (4)	0.106 (5)
C24	0.0474 (16)	0.0487 (16)	0.0452 (15)	0.0152 (12)	0.0095 (12)	0.0218 (13)
C25	0.0591 (19)	0.0501 (17)	0.0531 (17)	0.0097 (14)	0.0086 (14)	0.0179 (14)
C26	0.093 (3)	0.0420 (17)	0.075 (2)	0.0084 (16)	0.0313 (19)	0.0221 (16)
C27	0.112 (3)	0.0514 (19)	0.070 (2)	0.0149 (18)	0.041 (2)	0.0295 (17)
C28	0.092 (2)	0.0548 (19)	0.0534 (17)	0.0240 (16)	0.0267 (16)	0.0292 (15)
C29	0.0518 (17)	0.0464 (16)	0.0458 (15)	0.0145 (12)	0.0136 (12)	0.0227 (12)
C30	0.0551 (17)	0.0533 (17)	0.0378 (13)	0.0180 (13)	0.0091 (12)	0.0236 (12)
C31	0.091 (3)	0.059 (2)	0.0564 (19)	0.0043 (18)	0.0025 (18)	0.0159 (16)
C32	0.121 (4)	0.099 (3)	0.083 (3)	0.008 (3)	−0.039 (3)	0.024 (2)
C33	0.139 (4)	0.080 (3)	0.063 (2)	0.021 (2)	0.042 (2)	0.0110 (19)
C34	0.155 (4)	0.063 (2)	0.071 (2)	−0.002 (2)	0.005 (3)	0.004 (2)
C35	0.223 (5)	0.079 (2)	0.100 (3)	0.025 (2)	0.080 (3)	0.056 (2)
C36	0.222 (5)	0.080 (2)	0.126 (3)	0.027 (3)	0.078 (3)	0.063 (2)
C37	0.224 (5)	0.087 (2)	0.118 (3)	0.031 (3)	0.077 (3)	0.070 (2)
C38	0.217 (5)	0.089 (2)	0.116 (3)	0.026 (3)	0.086 (3)	0.066 (2)
C36A	0.223 (5)	0.084 (2)	0.124 (3)	0.029 (3)	0.076 (3)	0.067 (3)

C37A	0.221 (5)	0.090 (2)	0.117 (3)	0.028 (3)	0.082 (3)	0.068 (3)
C38A	0.219 (5)	0.085 (2)	0.121 (3)	0.024 (3)	0.082 (3)	0.066 (3)
C39	0.0624 (19)	0.0498 (17)	0.0451 (15)	0.0113 (14)	0.0098 (13)	0.0225 (13)
C40	0.063 (2)	0.0558 (19)	0.0617 (19)	0.0130 (15)	0.0015 (15)	0.0246 (15)
C41	0.081 (2)	0.065 (2)	0.063 (2)	0.0063 (18)	−0.0075 (17)	0.0180 (17)
C42	0.117 (3)	0.052 (2)	0.060 (2)	0.004 (2)	−0.001 (2)	0.0122 (17)
C43	0.162 (4)	0.053 (2)	0.080 (3)	0.031 (2)	−0.013 (3)	0.022 (2)
C44	0.122 (3)	0.055 (2)	0.063 (2)	0.022 (2)	−0.017 (2)	0.0209 (17)
C45	0.174 (5)	0.098 (4)	0.090 (3)	0.009 (3)	−0.024 (3)	−0.018 (3)
C46	0.298 (14)	0.053 (4)	0.101 (7)	0.046 (7)	0.024 (8)	0.025 (4)
C46A	0.301 (14)	0.057 (4)	0.101 (7)	0.039 (7)	0.025 (7)	0.025 (3)
N1	0.0582 (15)	0.0523 (14)	0.0473 (13)	0.0157 (11)	0.0083 (11)	0.0251 (11)
N2	0.0561 (14)	0.0433 (13)	0.0424 (12)	0.0138 (10)	0.0055 (10)	0.0192 (10)
N3	0.084 (3)	0.154 (4)	0.122 (3)	0.067 (2)	0.026 (2)	0.085 (3)
N4	0.184 (4)	0.057 (2)	0.083 (2)	−0.001 (2)	−0.016 (2)	0.0049 (18)
O1	0.0688 (13)	0.0738 (14)	0.0542 (11)	0.0259 (10)	0.0205 (10)	0.0417 (10)
O2	0.0741 (14)	0.0513 (11)	0.0418 (10)	0.0081 (9)	0.0097 (9)	0.0213 (9)
CO1	0.0632 (3)	0.0506 (3)	0.0427 (2)	0.01369 (18)	0.01155 (17)	0.02546 (18)

Geometric parameters (Å, º)

C1—O1	1.313 (3)	C25—C31	1.527 (4)
C1—C6	1.417 (4)	C26—C27	1.391 (5)
C1—C2	1.421 (4)	C26—H26	0.9300
C2—C3	1.380 (4)	C27—C28	1.362 (4)
C2—C7	1.535 (4)	C27—C35	1.532 (5)
C3—C4	1.402 (4)	C28—C29	1.415 (4)
C3—H3	0.9300	C28—H28	0.9300
C4—C5	1.353 (4)	C29—C30	1.428 (4)
C4—C11	1.524 (4)	C30—N2	1.295 (3)
C5—C6	1.417 (4)	C30—H30	0.9300
C5—H5	0.9300	C31—C32	1.528 (5)
C6—C15	1.414 (4)	C31—C33	1.540 (5)
C7—C9	1.513 (5)	C31—C34	1.556 (5)
C7—C8	1.522 (4)	C32—H32A	0.9600
C7—C10	1.537 (5)	C32—H32B	0.9600
C8—H8A	0.9600	C32—H32C	0.9600
C8—H8B	0.9600	C33—H33A	0.9600
C8—H8C	0.9600	C33—H33B	0.9600
C9—H9A	0.9600	C33—H33C	0.9600
C9—H9B	0.9600	C34—H34A	0.9600
C9—H9C	0.9600	C34—H34B	0.9600
C10—H10A	0.9600	C34—H34C	0.9600
C10—H10B	0.9600	C35—C37A	1.459 (9)
C10—H10C	0.9600	C35—C36	1.468 (7)
C11—C13A	1.512 (8)	C35—C38	1.513 (7)
C11—C12A	1.517 (8)	C35—C36A	1.514 (9)
C11—C14	1.530 (6)	C35—C37	1.594 (7)

C11—C13	1.540 (6)	C35—C38A	1.599 (9)
C11—C14A	1.547 (8)	C36—H36A	0.9600
C11—C12	1.551 (6)	C36—H36B	0.9600
C12—H12A	0.9600	C36—H36C	0.9600
C12—H12B	0.9600	C37—H37A	0.9600
C12—H12C	0.9600	C37—H37B	0.9600
C13—H13A	0.9600	C37—H37C	0.9600
C13—H13B	0.9600	C38—H38A	0.9600
C13—H13C	0.9600	C38—H38B	0.9600
C14—H14A	0.9600	C38—H38C	0.9600
C14—H14B	0.9600	C36A—H36D	0.9600
C14—H14C	0.9600	C36A—H36E	0.9600
C12A—H12D	0.9600	C36A—H36F	0.9600
C12A—H12E	0.9600	C37A—H37D	0.9600
C12A—H12F	0.9600	C37A—H37E	0.9600
C13A—H13D	0.9600	C37A—H37F	0.9600
C13A—H13E	0.9600	C38A—H38D	0.9600
C13A—H13F	0.9600	C38A—H38E	0.9600
C14A—H14D	0.9600	C38A—H38F	0.9600
C14A—H14E	0.9600	C39—C40	1.368 (4)
C14A—H14F	0.9600	C39—C44	1.381 (4)
C15—N1	1.307 (3)	C39—N2	1.426 (3)
C15—H15	0.9300	C40—C41	1.371 (4)
C16—C21	1.378 (4)	C40—H40	0.9300
C16—C17	1.395 (4)	C41—C42	1.381 (5)
C16—N1	1.428 (4)	C41—H41	0.9300
C17—C18	1.347 (5)	C42—C43	1.388 (5)
C17—H17	0.9300	C42—N4	1.395 (4)
C18—C19	1.403 (5)	C43—C44	1.369 (5)
C18—H18	0.9300	C43—H43	0.9300
C19—N3	1.368 (4)	C44—H44	0.9300
C19—C20	1.406 (5)	C45—N4	1.439 (6)
C20—C21	1.372 (4)	C45—H45A	0.9600
C20—H20	0.9300	C45—H45B	0.9600
C21—H21	0.9300	C45—H45C	0.9600
C22—N3	1.372 (6)	C46—N4	1.424 (10)
C22—H22A	0.9600	C46—H46A	0.9600
C22—H22B	0.9600	C46—H46B	0.9600
C22—H22C	0.9600	C46—H46C	0.9600
C23—N3	1.437 (6)	C46A—N4	1.445 (10)
C23—H23A	0.9600	C46A—H46D	0.9600
C23—H23B	0.9600	C46A—H46E	0.9600
C23—H23C	0.9600	C46A—H46F	0.9600
C24—O2	1.300 (3)	N1—CO1	1.980 (2)
C24—C25	1.418 (4)	N2—CO1	1.984 (2)
C24—C29	1.425 (4)	O1—CO1	1.8844 (19)
C25—C26	1.382 (4)	O2—CO1	1.8882 (19)

O1—C1—C6	121.6 (2)	C27—C28—H28	118.8
O1—C1—C2	120.1 (3)	C29—C28—H28	118.8
C6—C1—C2	118.2 (2)	C28—C29—C24	119.2 (3)
C3—C2—C1	118.5 (3)	C28—C29—C30	116.0 (2)
C3—C2—C7	121.0 (3)	C24—C29—C30	124.7 (2)
C1—C2—C7	120.5 (2)	N2—C30—C29	128.7 (2)
C2—C3—C4	124.5 (3)	N2—C30—H30	115.7
C2—C3—H3	117.8	C29—C30—H30	115.7
C4—C3—H3	117.8	C25—C31—C32	109.6 (3)
C5—C4—C3	116.2 (3)	C25—C31—C33	109.7 (3)
C5—C4—C11	124.0 (3)	C32—C31—C33	110.7 (3)
C3—C4—C11	119.8 (3)	C25—C31—C34	111.2 (3)
C4—C5—C6	123.2 (3)	C32—C31—C34	108.5 (3)
C4—C5—H5	118.4	C33—C31—C34	107.1 (3)
C6—C5—H5	118.4	C31—C32—H32A	109.5
C15—C6—C1	125.3 (3)	C31—C32—H32B	109.5
C15—C6—C5	115.4 (3)	H32A—C32—H32B	109.5
C1—C6—C5	119.3 (3)	C31—C32—H32C	109.5
C9—C7—C8	109.9 (3)	H32A—C32—H32C	109.5
C9—C7—C2	109.9 (3)	H32B—C32—H32C	109.5
C8—C7—C2	110.2 (3)	C31—C33—H33A	109.5
C9—C7—C10	108.0 (3)	C31—C33—H33B	109.5
C8—C7—C10	106.8 (3)	H33A—C33—H33B	109.5
C2—C7—C10	112.0 (3)	C31—C33—H33C	109.5
C7—C8—H8A	109.5	H33A—C33—H33C	109.5
C7—C8—H8B	109.5	H33B—C33—H33C	109.5
H8A—C8—H8B	109.5	C31—C34—H34A	109.5
C7—C8—H8C	109.5	C31—C34—H34B	109.5
H8A—C8—H8C	109.5	H34A—C34—H34B	109.5
H8B—C8—H8C	109.5	C31—C34—H34C	109.5
C7—C9—H9A	109.5	H34A—C34—H34C	109.5
C7—C9—H9B	109.5	H34B—C34—H34C	109.5
H9A—C9—H9B	109.5	C36—C35—C38	122.2 (6)
C7—C9—H9C	109.5	C37A—C35—C36A	126.9 (10)
H9A—C9—H9C	109.5	C37A—C35—C27	118.0 (6)
H9B—C9—H9C	109.5	C36—C35—C27	117.0 (5)
C7—C10—H10A	109.5	C38—C35—C27	107.6 (4)
C7—C10—H10B	109.5	C36A—C35—C27	107.2 (6)
H10A—C10—H10B	109.5	C36—C35—C37	97.9 (6)
C7—C10—H10C	109.5	C38—C35—C37	102.5 (6)
H10A—C10—H10C	109.5	C27—C35—C37	106.8 (4)
H10B—C10—H10C	109.5	C37A—C35—C38A	102.2 (10)
C13A—C11—C12A	110.5 (7)	C36A—C35—C38A	91.4 (9)
C13A—C11—C4	114.1 (6)	C27—C35—C38A	104.6 (5)
C12A—C11—C4	108.6 (5)	C35—C36—H36A	109.5
C4—C11—C14	113.7 (3)	C35—C36—H36B	109.5
C4—C11—C13	109.0 (4)	H36A—C36—H36B	109.5
C14—C11—C13	108.3 (5)	C35—C36—H36C	109.5

C13A—C11—C14A	105.7 (8)	H36A—C36—H36C	109.5
C12A—C11—C14A	110.2 (7)	H36B—C36—H36C	109.5
C4—C11—C14A	107.7 (5)	C35—C37—H37A	109.5
C4—C11—C12	108.8 (3)	C35—C37—H37B	109.5
C14—C11—C12	109.4 (4)	H37A—C37—H37B	109.5
C13—C11—C12	107.5 (4)	C35—C37—H37C	109.5
C11—C12—H12A	109.5	H37A—C37—H37C	109.5
C11—C12—H12B	109.5	H37B—C37—H37C	109.5
H12A—C12—H12B	109.5	C35—C38—H38A	109.5
C11—C12—H12C	109.5	C35—C38—H38B	109.5
H12A—C12—H12C	109.5	H38A—C38—H38B	109.5
H12B—C12—H12C	109.5	C35—C38—H38C	109.5
C11—C13—H13A	109.5	H38A—C38—H38C	109.5
C11—C13—H13B	109.5	H38B—C38—H38C	109.5
H13A—C13—H13B	109.5	C35—C36A—H36D	109.5
C11—C13—H13C	109.5	C35—C36A—H36E	109.5
H13A—C13—H13C	109.5	H36D—C36A—H36E	109.5
H13B—C13—H13C	109.5	C35—C36A—H36F	109.5
C11—C14—H14A	109.5	H36D—C36A—H36F	109.5
C11—C14—H14B	109.5	H36E—C36A—H36F	109.5
H14A—C14—H14B	109.5	C35—C37A—H37D	109.5
C11—C14—H14C	109.5	C35—C37A—H37E	109.5
H14A—C14—H14C	109.5	H37D—C37A—H37E	109.5
H14B—C14—H14C	109.5	C35—C37A—H37F	109.5
C11—C12A—H12D	109.5	H37D—C37A—H37F	109.5
C11—C12A—H12E	109.5	H37E—C37A—H37F	109.5
H12D—C12A—H12E	109.5	C35—C38A—H38D	109.5
C11—C12A—H12F	109.5	C35—C38A—H38E	109.5
H12D—C12A—H12F	109.5	H38D—C38A—H38E	109.5
H12E—C12A—H12F	109.5	C35—C38A—H38F	109.5
C11—C13A—H13D	109.5	H38D—C38A—H38F	109.5
C11—C13A—H13E	109.5	H38E—C38A—H38F	109.5
H13D—C13A—H13E	109.5	C40—C39—C44	117.7 (3)
C11—C13A—H13F	109.5	C40—C39—N2	122.9 (3)
H13D—C13A—H13F	109.5	C44—C39—N2	119.4 (3)
H13E—C13A—H13F	109.5	C39—C40—C41	121.8 (3)
C11—C14A—H14D	109.5	C39—C40—H40	119.1
C11—C14A—H14E	109.5	C41—C40—H40	119.1
H14D—C14A—H14E	109.5	C40—C41—C42	121.0 (3)
C11—C14A—H14F	109.5	C40—C41—H41	119.5
H14D—C14A—H14F	109.5	C42—C41—H41	119.5
H14E—C14A—H14F	109.5	C41—C42—C43	116.9 (3)
N1—C15—C6	129.0 (3)	C41—C42—N4	121.6 (4)
N1—C15—H15	115.5	C43—C42—N4	121.4 (4)
C6—C15—H15	115.5	C44—C43—C42	121.8 (3)
C21—C16—C17	117.5 (3)	C44—C43—H43	119.1
C21—C16—N1	119.0 (3)	C42—C43—H43	119.1
C17—C16—N1	123.4 (3)	C43—C44—C39	120.7 (3)

C18—C17—C16	121.7 (3)	C43—C44—H44	119.7
C18—C17—H17	119.1	C39—C44—H44	119.7
C16—C17—H17	119.1	N4—C45—H45A	109.5
C17—C18—C19	121.8 (3)	N4—C45—H45B	109.5
C17—C18—H18	119.1	H45A—C45—H45B	109.5
C19—C18—H18	119.1	N4—C45—H45C	109.5
N3—C19—C18	121.8 (4)	H45A—C45—H45C	109.5
N3—C19—C20	121.9 (4)	H45B—C45—H45C	109.5
C18—C19—C20	116.3 (3)	N4—C46—H46A	109.5
C21—C20—C19	121.3 (3)	N4—C46—H46B	109.5
C21—C20—H20	119.4	H46A—C46—H46B	109.5
C19—C20—H20	119.4	N4—C46—H46C	109.5
C20—C21—C16	121.3 (3)	H46A—C46—H46C	109.5
C20—C21—H21	119.3	H46B—C46—H46C	109.5
C16—C21—H21	119.3	N4—C46A—H46D	109.5
N3—C22—H22A	109.5	N4—C46A—H46E	109.5
N3—C22—H22B	109.5	H46D—C46A—H46E	109.5
H22A—C22—H22B	109.5	N4—C46A—H46F	109.5
N3—C22—H22C	109.5	H46D—C46A—H46F	109.5
H22A—C22—H22C	109.5	H46E—C46A—H46F	109.5
H22B—C22—H22C	109.5	C15—N1—C16	118.8 (2)
N3—C23—H23A	109.5	C15—N1—CO1	118.8 (2)
N3—C23—H23B	109.5	C16—N1—CO1	122.19 (18)
H23A—C23—H23B	109.5	C30—N2—C39	117.2 (2)
N3—C23—H23C	109.5	C30—N2—CO1	120.48 (18)
H23A—C23—H23C	109.5	C39—N2—CO1	122.15 (17)
H23B—C23—H23C	109.5	C19—N3—C22	122.3 (4)
O2—C24—C25	119.9 (2)	C19—N3—C23	120.8 (4)
O2—C24—C29	121.3 (2)	C22—N3—C23	116.5 (4)
C25—C24—C29	118.7 (2)	C42—N4—C45	119.6 (4)
C26—C25—C24	117.8 (3)	C42—N4—C46A	121.1 (5)
C26—C25—C31	122.3 (3)	C45—N4—C46A	118.3 (6)
C24—C25—C31	119.8 (3)	C1—O1—CO1	126.92 (18)
C25—C26—C27	124.9 (3)	C24—O2—CO1	129.44 (17)
C25—C26—H26	117.5	O1—CO1—O2	117.06 (9)
C27—C26—H26	117.5	O1—CO1—N1	96.23 (9)
C28—C27—C26	116.9 (3)	O2—CO1—N1	112.64 (9)
C28—C27—C35	121.2 (3)	O1—CO1—N2	119.77 (9)
C26—C27—C35	121.9 (3)	O2—CO1—N2	95.20 (8)
C27—C28—C29	122.4 (3)	N1—CO1—N2	117.31 (9)
O1—C1—C2—C3	−178.0 (3)	C25—C24—C29—C30	178.6 (3)
C6—C1—C2—C3	2.5 (4)	C28—C29—C30—N2	174.1 (3)
O1—C1—C2—C7	3.1 (4)	C24—C29—C30—N2	−3.2 (5)
C6—C1—C2—C7	−176.4 (3)	C26—C25—C31—C32	−116.3 (4)
C1—C2—C3—C4	−1.6 (4)	C24—C25—C31—C32	62.8 (4)
C7—C2—C3—C4	177.3 (3)	C26—C25—C31—C33	122.0 (4)
C2—C3—C4—C5	0.2 (5)	C24—C25—C31—C33	−58.9 (4)

C2—C3—C4—C11	−179.6 (3)	C26—C25—C31—C34	3.7 (5)
C3—C4—C5—C6	0.2 (5)	C24—C25—C31—C34	−177.2 (3)
C11—C4—C5—C6	180.0 (3)	C28—C27—C35—C37A	−27.5 (11)
O1—C1—C6—C15	−2.0 (5)	C26—C27—C35—C37A	152.6 (10)
C2—C1—C6—C15	177.5 (3)	C28—C27—C35—C36	157.3 (7)
O1—C1—C6—C5	178.3 (3)	C26—C27—C35—C36	−22.6 (9)
C2—C1—C6—C5	−2.2 (4)	C28—C27—C35—C38	−60.5 (7)
C4—C5—C6—C15	−178.8 (3)	C26—C27—C35—C38	119.6 (6)
C4—C5—C6—C1	0.9 (5)	C28—C27—C35—C36A	123.7 (8)
C3—C2—C7—C9	120.3 (3)	C26—C27—C35—C36A	−56.2 (9)
C1—C2—C7—C9	−60.8 (4)	C28—C27—C35—C37	48.9 (6)
C3—C2—C7—C8	−118.5 (3)	C26—C27—C35—C37	−131.0 (5)
C1—C2—C7—C8	60.4 (3)	C28—C27—C35—C38A	−140.2 (6)
C3—C2—C7—C10	0.2 (4)	C26—C27—C35—C38A	39.9 (7)
C1—C2—C7—C10	179.1 (3)	C44—C39—C40—C41	−1.1 (5)
C5—C4—C11—C13A	−151.0 (7)	N2—C39—C40—C41	178.9 (3)
C3—C4—C11—C13A	28.8 (8)	C39—C40—C41—C42	−0.8 (5)
C5—C4—C11—C12A	85.3 (8)	C40—C41—C42—C43	0.8 (6)
C3—C4—C11—C12A	−94.9 (8)	C40—C41—C42—N4	−179.7 (4)
C5—C4—C11—C14	−1.4 (6)	C41—C42—C43—C44	1.1 (7)
C3—C4—C11—C14	178.4 (4)	N4—C42—C43—C44	−178.4 (4)
C5—C4—C11—C13	−122.3 (5)	C42—C43—C44—C39	−3.0 (7)
C3—C4—C11—C13	57.6 (5)	C40—C39—C44—C43	3.0 (6)
C5—C4—C11—C14A	−34.0 (8)	N2—C39—C44—C43	−177.1 (4)
C3—C4—C11—C14A	145.8 (7)	C6—C15—N1—C16	179.2 (3)
C5—C4—C11—C12	120.8 (5)	C6—C15—N1—CO1	−5.0 (4)
C3—C4—C11—C12	−59.4 (5)	C21—C16—N1—C15	146.7 (3)
C1—C6—C15—N1	−2.1 (5)	C17—C16—N1—C15	−34.3 (4)
C5—C6—C15—N1	177.6 (3)	C21—C16—N1—CO1	−29.0 (3)
C21—C16—C17—C18	−1.9 (4)	C17—C16—N1—CO1	150.0 (2)
N1—C16—C17—C18	179.1 (3)	C29—C30—N2—C39	−179.9 (3)
C16—C17—C18—C19	1.3 (5)	C29—C30—N2—CO1	4.9 (4)
C17—C18—C19—N3	179.3 (3)	C40—C39—N2—C30	−46.4 (4)
C17—C18—C19—C20	−1.1 (5)	C44—C39—N2—C30	133.7 (3)
N3—C19—C20—C21	−178.8 (3)	C40—C39—N2—CO1	128.7 (3)
C18—C19—C20—C21	1.5 (5)	C44—C39—N2—CO1	−51.2 (4)
C19—C20—C21—C16	−2.3 (5)	C18—C19—N3—C22	178.2 (4)
C17—C16—C21—C20	2.4 (4)	C20—C19—N3—C22	−1.4 (6)
N1—C16—C21—C20	−178.6 (3)	C18—C19—N3—C23	5.4 (6)
O2—C24—C25—C26	178.2 (3)	C20—C19—N3—C23	−174.2 (4)
C29—C24—C25—C26	−1.6 (4)	C41—C42—N4—C45	5.4 (7)
O2—C24—C25—C31	−0.9 (4)	C43—C42—N4—C45	−175.1 (5)
C29—C24—C25—C31	179.3 (3)	C41—C42—N4—C46A	−162.7 (14)
C24—C25—C26—C27	0.7 (5)	C43—C42—N4—C46A	16.7 (15)
C31—C25—C26—C27	179.8 (3)	C6—C1—O1—CO1	13.7 (4)
C25—C26—C27—C28	0.4 (6)	C2—C1—O1—CO1	−165.78 (19)
C25—C26—C27—C35	−179.6 (4)	C25—C24—O2—CO1	−176.91 (19)
C26—C27—C28—C29	−0.7 (5)	C29—C24—O2—CO1	2.9 (4)

C35—C27—C28—C29	179.4 (4)	C1—O1—CO1—O2	102.9 (2)
C27—C28—C29—C24	−0.3 (5)	C1—O1—CO1—N1	−16.5 (2)
C27—C28—C29—C30	−177.7 (3)	C1—O1—CO1—N2	−143.0 (2)
O2—C24—C29—C28	−178.4 (3)	C24—O2—CO1—O1	126.3 (2)
C25—C24—C29—C28	1.4 (4)	C24—O2—CO1—N1	−123.5 (2)
O2—C24—C29—C30	−1.3 (4)	C24—O2—CO1—N2	−1.1 (2)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*C*···O1	0.96	2.38	3.007 (4)	123
C9—H9*A*···O1	0.96	2.28	2.953 (4)	126
C32—H32*C*···O2	0.96	2.33	2.974 (4)	124
C33—H33*C*···O2	0.96	2.28	2.925 (4)	124
C45—H45*B*···*Cg*^{i}	0.96	2.96	3.914 (5)	171

Symmetry code: (i) −*x*, −*y*, −*z*.