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1-(3,4-Dimethoxyphenyl)-3-[4-(dimethylamino)phenyl]prop-2-en-1-one

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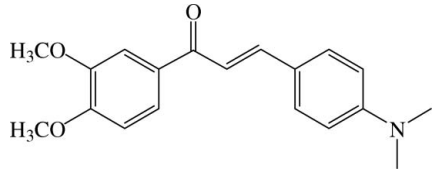
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.128; data-to-parameter ratio = 11.3.

The title compound, $C_{19}H_{21}NO_3$, is a chalcone derivative which crystallizes with four independent molecules in the asymmetric unit. The dihedral angles between the two benzene rings are in the range 31.73 (14)–38.62 (16)° in the four molecules. In all the molecules, the two methoxy groups deviate slightly from the mean planes of the attached benzene rings. One methyl of the dimethylamino group is coplanar while the other is not coplanar with the attached benzene rings in two of the molecules, whereas in the other two molecules both methyl groups of the dimethylamino group are twisted out of the planes of the attached benzene rings. Weak C—H···O intramolecular interactions involving the enone unit generate S(5) ring motifs. In the crystal structure, the molecules are arranged into chains along the c axis. These chains are stacked along the b axis. The crystal structure is stabilized by weak C—H···O intra- and intermolecular interactions, together with C—H···π interactions.

Related literature

For hydrogen-bond motifs, see Bernstein *et al.* (1995). For values of bond lengths, see Allen *et al.* (1987). For non-linear optical properties, see, for example, Williams (1984). For related structures, see, for example, Patil, Dharmaprakash *et al.* (2006, 2007); Patil, Teh *et al.* (2006); Fun, Chantrapromma *et al.* (2007); Fun, Patil *et al.* (2007); Patil, Chantrapromma *et al.* (2007); Patil, Ng *et al.* (2007); Patil, Rosli *et al.* (2007); Shettigar *et al.* (2006).



Experimental

Crystal data

$C_{19}H_{21}NO_3$
M_r = 311.37
Monoclinic, Pc
a = 10.8945 (2) Å
b = 9.7106 (2) Å
c = 32.6158 (5) Å
β = 109.412 (1)°
V = 3254.35 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100.0 (1) K
0.46 × 0.41 × 0.33 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.962, T_{max} = 0.973
82540 measured reflections
9514 independent reflections
7984 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.128
S = 1.05
9514 reflections
845 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C16C—H16I···O2D^{i}	0.96	2.40	3.306 (4)	157
C16D—H16K···O1B^{ii}	0.96	2.60	3.489 (5)	154
C16D—H16L···O2C^{i}	0.96	2.57	3.460 (4)	155
C18B—H18D···O1C^{iii}	0.96	2.58	3.283 (5)	130
C18C—H18G···O1A^{iv}	0.96	2.56	3.320 (5)	136
C19A—H19B···O2B^{ii}	0.96	2.60	3.446 (5)	147
C2B—H2B···$Cg1$	0.93	2.92	3.737 (3)	148
C2D—H2D···$Cg3$	0.93	2.91	3.718 (2)	147
C5A—H5A···$Cg4$	0.93	2.91	3.559 (3)	128
C5B—H5B···$Cg1^{v}$	0.93	2.72	3.466 (3)	138
C5C—H5C···$Cg2$	0.93	2.92	3.559 (3)	128
C5D—H5D···$Cg3^{ii}$	0.93	2.73	3.481 (3)	139
C14A—H14A···$Cg7^{vi}$	0.93	3.03	3.742 (4)	135
C14B—H14B···$Cg8^{vi}$	0.93	3.05	3.773 (4)	136
C14C—H14C···$Cg6^{vii}$	0.93	2.96	3.676 (4)	135
C14D—H14D···$Cg5^{viii}$	0.93	3.17	3.875 (4)	134
C18A—H18B···$Cg6$	0.96	2.67	3.480 (4)	142
C18B—H18E···$Cg5^{v}$	0.96	2.83	3.683 (4)	149
C18C—H18I···$Cg8$	0.96	2.82	3.639 (4)	144
C18D—H18L···$Cg7^{ii}$	0.96	2.70	3.505 (4)	142

Symmetry codes: (i) $x, -y+1, z-\frac{1}{2}$; (ii) $x, y+1, z$; (iii) $x, -y, z-\frac{1}{2}$; (iv) $x, -y+1, z+\frac{1}{2}$; (v) $x, y-1, z$; (vi) $x-1, -y+1, z-\frac{1}{2}$; (vii) $x+1, -y, z+\frac{1}{2}$; (viii) $x+1, -y+1, z+\frac{1}{2}$. $Cg1$, $Cg2$, $Cg3$, $Cg4$, $Cg5$, $Cg6$, $Cg7$ and $Cg8$ are the centroids of rings C1A–C6A, C1B–C6B, C1C–C6C, C1D–C6D, C10A–C15A, C10B–C15B, C10C–C15C and C10D–C15D, respectively.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used

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to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2156).

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supplementary materials

Acta Cryst. (2007). E**63**, o3253-o3254 [**doi:10.1107/S1600536807029029**]

1-(3,4-Dimethoxyphenyl)-3-[4-(dimethylamino)phenyl]prop-2-en-1-one

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Comment

Chalcone derivatives are important NLO materials with excellent blue light transmittance and good crystallizability (Patil, Teh *et al.*, 2006; Patil, Dharmaprakash *et al.*, 2006; 2007). In a continuation of our studies on the structural and non-linear optical properties of chalcone derivatives (Patil, Dharmaprakash *et al.*, 2006; 2007; Patil, Teh *et al.*, 2006; Fun, Chantrapromma *et al.*, 2007; Fun, Patil *et al.*, 2007; Patil, Chantrapromma *et al.*, 2007; Patil, Ng *et al.*, 2007; Patil, Rosli *et al.*, 2007; Shettigar *et al.*, 2006), the crystal structure determination of the title compound was undertaken in order to establish the three dimensional structure. Since the title compound crystallizes in a non-centrosymmetric monoclinic space group, *Pc*, it should exhibit second-order non-linear optical properties (Williams, 1984).

In the asymmetric unit of the title compound (Fig. 1), there are four independent molecules *A*, *B*, *C* and *D*. Bond lengths and angles show normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Patil, Teh *et al.*, 2006; Patil, Dharmaprakash *et al.*, 2006; 2007; Shettigar *et al.*, 2006; Patil, Ng *et al.*, 2007; Patil, Chantrapromma *et al.*, 2007). The dihedral angles between the two benzene rings are 32.54 (15)°, 38.62 (16)°, 31.73 (14)° and 37.38 (16)° in molecules *A*, *B*, *C* and *D*, respectively. In molecule *A*, the least-squares plane through the O1/C7/C8/C9/C10 group makes dihedral angles of 16.84 (16)° and 16.74 (18)° with the C1–C6 and C10–C15 benzene rings, respectively; the corresponding values are 37.14 (16)° and 4.30 (17)° in molecule *B*, 17.88 (15)° and 14.93 (17)° in molecule *C*, 36.80 (17)° and 5.29 (17)° in molecule *D*. The two methoxy groups deviate slightly from the mean planes of the attached benzene rings, with the C18/O2/C12/C13 torsion angles of 171.5 (3)°, 167.6 (3)°, −168.6 (3)° and −169.1 (3)° in molecules *A*, *B*, *C* and *D*, respectively. The C19/O3/C13/C12 torsion angles are −172.3 (3)°, −171.2 (3)°, 169.7 (3)° and 173.7 (3)° in molecules *A*, *B*, *C* and *D*, respectively. The orientations of the dimethylamino groups can be described by the torsion angles C16/N1/C3/C2 = −179.1 (3)° and C17/N1/C3/N2 = −4.5 (5)° in molecule *A* [the corresponding values are −168.6 (3)° and −16.4 (5)° in molecule *B*, −179.3 (3)° and 3.0 (5)° in molecule *C*, 169.4 (3)° and 15.0 (5)° in molecule *D*], indicating that one methyl of the dimethylamino group is coplanar while the other is not coplanar with the attached benzene rings in molecules *A* and *C*, whereas in molecules *B* and *D* both methyl groups of dimethylamino are twisted out of the planes of the attached benzene rings.

In the structure of the title compound, weak C7A—H7A···O1A, C7B—H7B···O1B, C7C—H7C···O1C, C7D—H7D···O1D and C11B···H11B···O1B intramolecular interactions generate S(5) ring motifs (Bernstein *et al.*, 1995) (Table 1). The molecules are arranged into chains along the *c* axis. These chains are stacked along the *b* axis. The crystal structure is stabilized by weak C—H···O intra- and intermolecular interactions, together with C—H···π interactions (Table 1); *Cg*1, *Cg*2, *Cg*3, *Cg*4, *Cg*5, *Cg*6, *Cg*7 and *Cg*8 are the centroids of rings C1A–C6A, C1B–C6B, C1C–C6C, C1D–C6D, C10A–C15A, C10B–C15B, C10C–C15C and C10D–C15D, respectively.

Experimental

The experimental procedure was similar to that previously reported (Patil, Chantrapromma *et al.*, 2007). The actual quantities used for the preparation of the title compound were 10 ml of 20% NaOH aqueous solution, 4-dimethylaminobenzaldehyde

(0.01 mol) in methanol (30 ml), and 3, 4-dimethoxyacetophenone (0.01 mol) in methanol (30 ml). Single crystals of the title compound suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature.

Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å. The U_{iso} values were set equal to $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. 9399 Friedel pairs were merged as there is no significant anomalous dispersion to determine the absolute structure.

Figures

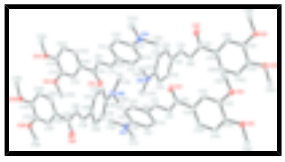


Fig. 1. The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering. H atoms are omitted for clarity.

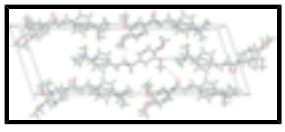


Fig. 2. The crystal packing of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

1-(3,4-Dimethoxyphenyl)-3-[4-(dimethylamino)phenyl]prop-2-en-1-one

Crystal data

$C_{19}H_{21}NO_3$	F_{000} = 1328
M_r = 311.37	D_x = 1.271 Mg m^{-3}
Monoclinic, *Pc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P -2yc	Cell parameters from 9514 reflections
a = 10.8945 (2) Å	θ = 1.3–30.0º
b = 9.7106 (2) Å	μ = 0.09 mm^{-1}
c = 32.6158 (5) Å	*T* = 100.0 (1) K
β = 109.412 (1)º	Block, colorless
V = 3254.35 (10) Å^3	0.46 × 0.41 × 0.33 mm
Z = 8	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	9514 independent reflections
Radiation source: fine-focus sealed tube	7984 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 30.0º
T = 100.0(1) K	θ_{min} = 1.3º
ω scans	*h* = −15→15

Absorption correction: multi-scan (SADABS; Bruker, 2005)

T_{min} = 0.962, T_{max} = 0.973

82540 measured reflections

k = −13→13

l = −45→45

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.044

$wR(F^2)$ = 0.128

S = 1.05

9514 reflections

845 parameters

2 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

$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 0.7226P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.004

$\Delta\rho_{max}$ = 0.43 e Å^{-3}

$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Extinction correction: none

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 $F^2 > 2$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}
O1A	0.2184 (3)	0.3576 (3)	0.19446 (8)	0.0281 (6)
O2A	0.0282 (2)	0.2504 (2)	0.03314 (7)	0.0205 (5)
O3A	−0.1536 (2)	0.4265 (3)	0.00106 (8)	0.0219 (5)
N1A	−0.0237 (3)	0.6424 (3)	0.39943 (10)	0.0205 (6)
C1A	−0.0466 (2)	0.5604 (3)	0.28688 (8)	0.0195 (5)
H1A	−0.1096	0.5567	0.2594	0.023*
C2A	−0.0830 (3)	0.5998 (3)	0.32199 (9)	0.0203 (5)
H2A	−0.1692	0.6225	0.3178	0.024*
C3A	0.0108 (3)	0.6058 (3)	0.36451 (11)	0.0175 (6)
C4A	0.1401 (3)	0.5717 (3)	0.36894 (8)	0.0188 (4)
H4A	0.2039	0.5758	0.3962	0.023*

C5A	0.1737 (2)	0.5323 (2)	0.33333 (8)	0.0186 (4)
H5A	0.2598	0.5094	0.3373	0.022*
C6A	0.0819 (3)	0.5259 (3)	0.29138 (10)	0.0175 (6)
C7A	0.1254 (3)	0.4812 (3)	0.25591 (10)	0.0189 (6)
H7A	0.2104	0.4486	0.2638	0.023*
C8A	0.0578 (3)	0.4814 (3)	0.21323 (10)	0.0198 (6)
H8A	−0.0245	0.5214	0.2033	0.024*
C9A	0.1126 (3)	0.4189 (4)	0.18204 (11)	0.0188 (6)
C10A	0.0367 (4)	0.4266 (4)	0.13441 (11)	0.0186 (6)
C11A	0.0706 (3)	0.3348 (4)	0.10696 (10)	0.0164 (6)
H11A	0.1381	0.2726	0.1187	0.020*
C12A	0.0051 (3)	0.3350 (3)	0.06236 (11)	0.0181 (6)
C13A	−0.0975 (3)	0.4307 (3)	0.04503 (10)	0.0160 (6)
C14A	−0.1309 (3)	0.5219 (3)	0.07285 (12)	0.0194 (6)
H14A	−0.1978	0.5852	0.0617	0.023*
C15A	−0.0637 (3)	0.5174 (4)	0.11704 (11)	0.0186 (6)
H15A	−0.0872	0.5773	0.1354	0.022*
C16A	0.0752 (3)	0.6496 (3)	0.44262 (9)	0.0240 (5)
H16A	0.1218	0.5639	0.4489	0.036*
H16B	0.0339	0.6664	0.4640	0.036*
H16C	0.1348	0.7230	0.4433	0.036*
C17A	−0.1547 (3)	0.6859 (4)	0.39406 (11)	0.0374 (7)
H17A	−0.2144	0.6132	0.3808	0.056*
H17B	−0.1754	0.7662	0.3759	0.056*
H17C	−0.1615	0.7074	0.4220	0.056*
C18A	0.1414 (3)	0.1660 (4)	0.04795 (11)	0.0229 (6)
H18A	0.1511	0.1158	0.0239	0.034*
H18B	0.1327	0.1024	0.0694	0.034*
H18C	0.2165	0.2229	0.0606	0.034*
C19A	−0.2460 (4)	0.5325 (4)	−0.01832 (12)	0.0250 (7)
H19A	−0.2708	0.5266	−0.0494	0.037*
H19B	−0.2076	0.6209	−0.0088	0.037*
H19C	−0.3215	0.5210	−0.0097	0.037*
O1B	0.2013 (3)	−0.1813 (3)	0.18798 (8)	0.0321 (6)
O2B	0.0047 (2)	−0.2380 (3)	0.02555 (8)	0.0229 (5)
O3B	−0.1786 (2)	−0.0577 (3)	−0.00111 (8)	0.0225 (5)
N1B	−0.0187 (3)	0.1402 (3)	0.39488 (11)	0.0226 (6)
C1B	0.0394 (3)	0.1339 (3)	0.28945 (9)	0.0205 (5)
H1B	0.0303	0.1921	0.2660	0.025*
C2B	0.0091 (2)	0.1832 (3)	0.32470 (9)	0.0198 (5)
H2B	−0.0185	0.2738	0.3247	0.024*
C3B	0.0195 (3)	0.0973 (4)	0.36088 (11)	0.0193 (7)
C4B	0.0685 (3)	−0.0364 (3)	0.36010 (9)	0.0255 (5)
H4B	0.0803	−0.0944	0.3838	0.031*
C5B	0.0993 (3)	−0.0829 (3)	0.32467 (9)	0.0248 (5)
H5B	0.1316	−0.1718	0.3252	0.030*
C6B	0.0835 (3)	−0.0011 (3)	0.28810 (10)	0.0197 (6)
C7B	0.1145 (3)	−0.0601 (3)	0.25157 (10)	0.0217 (6)
H7B	0.1604	−0.1427	0.2570	0.026*

C8B	0.0851 (3)	−0.0101 (4)	0.21119 (11)	0.0228 (7)
H8B	0.0463	0.0759	0.2043	0.027*
C9B	0.1148 (3)	−0.0926 (4)	0.17769 (11)	0.0214 (7)
C10B	0.0361 (3)	−0.0737 (4)	0.13050 (11)	0.0191 (6)
C11B	0.0594 (3)	−0.1639 (4)	0.10077 (11)	0.0184 (6)
H11B	0.1241	−0.2303	0.1106	0.022*
C12B	−0.0122 (3)	−0.1567 (3)	0.05660 (11)	0.0183 (6)
C13B	−0.1121 (3)	−0.0582 (3)	0.04240 (11)	0.0172 (6)
C14B	−0.1360 (3)	0.0323 (4)	0.07259 (12)	0.0195 (6)
H14B	−0.2013	0.0983	0.0634	0.023*
C15B	−0.0617 (3)	0.0225 (4)	0.11609 (11)	0.0188 (6)
H15B	−0.0782	0.0820	0.1360	0.023*
C16B	0.0166 (4)	0.0582 (3)	0.43435 (10)	0.0357 (7)
H16D	−0.0152	−0.0340	0.4274	0.053*
H16E	−0.0214	0.0980	0.4543	0.053*
H16F	0.1096	0.0565	0.4475	0.053*
C17B	−0.0386 (3)	0.2871 (3)	0.40042 (10)	0.0283 (6)
H17D	−0.0986	0.3236	0.3740	0.042*
H17E	0.0430	0.3346	0.4073	0.042*
H17F	−0.0733	0.2995	0.4236	0.042*
C18B	0.1205 (3)	−0.3197 (4)	0.03682 (12)	0.0266 (7)
H18D	0.1264	−0.3640	0.0112	0.040*
H18E	0.1177	−0.3882	0.0577	0.040*
H18F	0.1951	−0.2616	0.0491	0.040*
C19B	−0.2680 (4)	0.0535 (4)	−0.01769 (12)	0.0270 (7)
H19D	−0.3014	0.0486	−0.0488	0.041*
H19E	−0.2239	0.1396	−0.0089	0.041*
H19F	−0.3387	0.0465	−0.0064	0.041*
O1C	0.3242 (3)	0.3951 (3)	0.48521 (8)	0.0286 (6)
O2C	0.5207 (2)	0.4875 (3)	0.64804 (8)	0.0212 (5)
O3C	0.7110 (2)	0.3146 (3)	0.67663 (8)	0.0210 (5)
N1C	0.5528 (3)	0.1027 (3)	0.27746 (11)	0.0229 (6)
C1C	0.5807 (3)	0.1868 (3)	0.39053 (8)	0.0199 (5)
H1C	0.6447	0.1911	0.4178	0.024*
C2C	0.6151 (3)	0.1474 (3)	0.35520 (9)	0.0212 (5)
H2C	0.7012	0.1252	0.3590	0.025*
C3C	0.5202 (4)	0.1403 (3)	0.31297 (11)	0.0184 (6)
C4C	0.3910 (2)	0.1760 (2)	0.30889 (8)	0.0189 (5)
H4C	0.3268	0.1735	0.2817	0.023*
C5C	0.3592 (2)	0.2142 (2)	0.34453 (8)	0.0193 (5)
H5C	0.2731	0.2367	0.3407	0.023*
C6C	0.4512 (3)	0.2209 (3)	0.38660 (10)	0.0182 (6)
C7C	0.4108 (3)	0.2674 (3)	0.42221 (10)	0.0199 (6)
H7C	0.3262	0.3008	0.4147	0.024*
C8C	0.4801 (3)	0.2686 (3)	0.46489 (10)	0.0196 (6)
H8C	0.5627	0.2296	0.4745	0.024*
C9C	0.4266 (4)	0.3308 (4)	0.49645 (11)	0.0211 (7)
C10C	0.5057 (3)	0.3215 (3)	0.54354 (11)	0.0161 (6)
C11C	0.4735 (3)	0.4099 (3)	0.57307 (11)	0.0183 (6)

H11C	0.4043	0.4710	0.5628	0.022*
C12C	0.5435 (3)	0.4059 (3)	0.61652 (11)	0.0163 (6)
C13C	0.6476 (3)	0.3107 (3)	0.63270 (11)	0.0175 (6)
C14C	0.6779 (3)	0.2237 (3)	0.60477 (11)	0.0178 (6)
H14C	0.7458	0.1612	0.6154	0.021*
C15C	0.6075 (3)	0.2272 (3)	0.55993 (12)	0.0179 (6)
H15C	0.6287	0.1668	0.5412	0.021*
C16C	0.4548 (3)	0.0976 (3)	0.23450 (9)	0.0252 (5)
H16G	0.4100	0.1842	0.2283	0.038*
H16H	0.3937	0.0255	0.2336	0.038*
H16I	0.4961	0.0797	0.2132	0.038*
C17C	0.6846 (3)	0.0624 (4)	0.28227 (11)	0.0372 (7)
H17G	0.7431	0.1359	0.2957	0.056*
H17H	0.6909	0.0430	0.2542	0.056*
H17I	0.7073	−0.0185	0.3001	0.056*
C18C	0.4028 (4)	0.5656 (4)	0.63452 (13)	0.0270 (7)
H18G	0.3944	0.6151	0.6589	0.040*
H18H	0.3301	0.5045	0.6232	0.040*
H18I	0.4047	0.6296	0.6123	0.040*
C19C	0.8005 (4)	0.2048 (4)	0.69443 (12)	0.0258 (7)
H19G	0.8313	0.2111	0.7256	0.039*
H19H	0.8728	0.2116	0.6839	0.039*
H19I	0.7574	0.1181	0.6857	0.039*
O1D	0.3263 (3)	0.9259 (3)	0.48468 (9)	0.0309 (6)
O2D	0.5134 (2)	1.0042 (3)	0.64606 (8)	0.0207 (5)
O3D	0.6913 (3)	0.8210 (3)	0.67617 (8)	0.0232 (5)
N1D	0.5476 (3)	0.6017 (3)	0.27921 (11)	0.0234 (6)
C1D	0.4941 (3)	0.6108 (3)	0.38553 (8)	0.0197 (5)
H1D	0.5043	0.5531	0.4092	0.024*
C2D	0.5236 (2)	0.5615 (2)	0.35009 (8)	0.0192 (5)
H2D	0.5517	0.4711	0.3502	0.023*
C3D	0.5117 (4)	0.6460 (3)	0.31398 (11)	0.0189 (7)
C4D	0.4631 (3)	0.7807 (3)	0.31468 (9)	0.0268 (6)
H4D	0.4511	0.8384	0.2909	0.032*
C5D	0.4332 (3)	0.8275 (3)	0.35014 (9)	0.0251 (5)
H5D	0.4014	0.9166	0.3497	0.030*
C6D	0.4494 (3)	0.7449 (4)	0.38671 (10)	0.0196 (6)
C7D	0.4182 (3)	0.8042 (3)	0.42283 (11)	0.0215 (6)
H7D	0.3711	0.8859	0.4169	0.026*
C8D	0.4483 (3)	0.7569 (4)	0.46385 (11)	0.0215 (6)
H8D	0.4909	0.6731	0.4718	0.026*
C9D	0.4124 (3)	0.8402 (4)	0.49585 (11)	0.0204 (7)
C10D	0.4906 (3)	0.8260 (3)	0.54287 (10)	0.0161 (6)
C11D	0.4629 (3)	0.9200 (4)	0.57189 (11)	0.0179 (6)
H11D	0.3968	0.9845	0.5613	0.021*
C12D	0.5325 (3)	0.9169 (3)	0.61539 (11)	0.0158 (6)
C13D	0.6306 (3)	0.8167 (4)	0.63231 (11)	0.0195 (6)
C14D	0.6593 (3)	0.7258 (4)	0.60467 (11)	0.0192 (7)
H14D	0.7258	0.6619	0.6156	0.023*

C15D	0.5890 (3)	0.7284 (3)	0.55968 (12)	0.0206 (7)
H15D	0.6081	0.6653	0.5412	0.025*
C16D	0.5116 (4)	0.6850 (3)	0.23981 (10)	0.0358 (7)
H16J	0.5491	0.7752	0.2466	0.054*
H16K	0.4186	0.6927	0.2281	0.054*
H16L	0.5435	0.6422	0.2188	0.054*
C17D	0.5689 (3)	0.4571 (3)	0.27397 (10)	0.0292 (6)
H17J	0.6332	0.4227	0.2999	0.044*
H17K	0.5989	0.4446	0.2497	0.044*
H17L	0.4889	0.4078	0.2689	0.044*
C18D	0.4001 (3)	1.0900 (3)	0.63159 (12)	0.0231 (6)
H18J	0.3939	1.1436	0.6555	0.035*
H18K	0.3240	1.0335	0.6204	0.035*
H18L	0.4066	1.1504	0.6091	0.035*
C19D	0.7807 (4)	0.7130 (4)	0.69470 (13)	0.0271 (7)
H19J	0.8113	0.7215	0.7258	0.041*
H19K	0.8532	0.7188	0.6842	0.041*
H19L	0.7381	0.6257	0.6866	0.041*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0250 (11)	0.0387 (13)	0.0197 (11)	0.0097 (9)	0.0062 (9)	0.0022 (9)
O2A	0.0240 (11)	0.0233 (10)	0.0144 (10)	0.0045 (8)	0.0064 (8)	0.0011 (8)
O3A	0.0199 (11)	0.0254 (11)	0.0168 (10)	0.0055 (8)	0.0015 (8)	−0.0003 (8)
N1A	0.0175 (13)	0.0264 (14)	0.0181 (13)	−0.0028 (10)	0.0064 (10)	−0.0020 (10)
C1A	0.0177 (11)	0.0227 (11)	0.0152 (11)	−0.0002 (9)	0.0018 (9)	0.0002 (9)
C2A	0.0181 (11)	0.0234 (12)	0.0188 (12)	−0.0004 (9)	0.0054 (9)	−0.0003 (9)
C3A	0.0182 (14)	0.0178 (14)	0.0171 (14)	−0.0023 (10)	0.0067 (11)	0.0004 (10)
C4A	0.0197 (11)	0.0210 (11)	0.0135 (10)	−0.0030 (9)	0.0025 (9)	−0.0009 (8)
C5A	0.0177 (11)	0.0195 (11)	0.0172 (11)	−0.0012 (8)	0.0039 (9)	−0.0006 (9)
C6A	0.0197 (14)	0.0178 (13)	0.0160 (13)	−0.0026 (10)	0.0073 (11)	−0.0017 (10)
C7A	0.0198 (13)	0.0213 (14)	0.0163 (13)	−0.0021 (10)	0.0069 (10)	−0.0017 (10)
C8A	0.0225 (14)	0.0225 (13)	0.0157 (12)	0.0007 (10)	0.0080 (11)	−0.0014 (10)
C9A	0.0203 (14)	0.0213 (14)	0.0146 (14)	−0.0006 (11)	0.0056 (11)	−0.0013 (10)
C10A	0.0185 (14)	0.0196 (14)	0.0171 (14)	−0.0007 (11)	0.0051 (11)	0.0005 (11)
C11A	0.0184 (14)	0.0181 (13)	0.0131 (14)	0.0003 (10)	0.0056 (11)	0.0013 (10)
C12A	0.0184 (14)	0.0151 (12)	0.0213 (16)	−0.0013 (10)	0.0073 (12)	0.0003 (10)
C13A	0.0179 (14)	0.0187 (13)	0.0111 (13)	0.0004 (10)	0.0044 (10)	0.0018 (10)
C14A	0.0180 (13)	0.0177 (14)	0.0222 (16)	0.0024 (11)	0.0061 (11)	−0.0002 (11)
C15A	0.0214 (14)	0.0207 (15)	0.0154 (13)	−0.0001 (11)	0.0083 (11)	−0.0017 (11)
C16A	0.0283 (14)	0.0293 (13)	0.0140 (11)	−0.0033 (10)	0.0066 (10)	−0.0036 (9)
C17A	0.0244 (14)	0.064 (2)	0.0263 (15)	0.0071 (13)	0.0117 (12)	−0.0055 (14)
C18A	0.0230 (14)	0.0246 (14)	0.0221 (14)	0.0034 (11)	0.0090 (11)	−0.0014 (11)
C19A	0.0244 (15)	0.0247 (15)	0.0203 (15)	0.0043 (11)	0.0000 (12)	0.0020 (11)
O1B	0.0306 (12)	0.0449 (14)	0.0208 (11)	0.0109 (11)	0.0084 (9)	0.0057 (10)
O2B	0.0222 (11)	0.0248 (11)	0.0213 (11)	0.0037 (8)	0.0067 (9)	−0.0025 (8)
O3B	0.0230 (11)	0.0248 (11)	0.0163 (10)	0.0042 (8)	0.0021 (8)	0.0000 (8)

N1B	0.0266 (14)	0.0178 (12)	0.0251 (14)	0.0023 (10)	0.0108 (11)	0.0006 (10)
C1B	0.0181 (11)	0.0234 (12)	0.0169 (12)	−0.0041 (9)	0.0015 (9)	0.0037 (9)
C2B	0.0173 (11)	0.0193 (11)	0.0203 (12)	−0.0002 (8)	0.0026 (9)	0.0024 (9)
C3B	0.0152 (13)	0.0214 (15)	0.0204 (15)	−0.0011 (10)	0.0046 (12)	0.0017 (11)
C4B	0.0375 (15)	0.0210 (12)	0.0216 (12)	0.0019 (10)	0.0147 (11)	0.0059 (9)
C5B	0.0350 (14)	0.0182 (11)	0.0236 (13)	0.0014 (10)	0.0130 (11)	0.0028 (10)
C6B	0.0190 (13)	0.0210 (14)	0.0185 (13)	−0.0065 (10)	0.0055 (11)	0.0011 (11)
C7B	0.0226 (13)	0.0239 (15)	0.0185 (12)	−0.0047 (11)	0.0066 (10)	−0.0017 (11)
C8B	0.0220 (15)	0.0286 (14)	0.0155 (13)	−0.0037 (11)	0.0034 (11)	−0.0002 (10)
C9B	0.0195 (15)	0.0270 (16)	0.0175 (14)	−0.0047 (11)	0.0062 (11)	0.0003 (11)
C10B	0.0160 (13)	0.0233 (15)	0.0165 (14)	−0.0049 (11)	0.0036 (11)	0.0027 (11)
C11B	0.0185 (14)	0.0179 (13)	0.0188 (15)	−0.0015 (10)	0.0061 (11)	0.0019 (10)
C12B	0.0194 (14)	0.0184 (13)	0.0175 (14)	−0.0037 (10)	0.0065 (11)	0.0005 (10)
C13B	0.0168 (13)	0.0203 (14)	0.0142 (13)	−0.0019 (10)	0.0049 (11)	0.0002 (11)
C14B	0.0179 (13)	0.0193 (14)	0.0217 (15)	−0.0004 (11)	0.0069 (11)	−0.0024 (11)
C15B	0.0205 (14)	0.0225 (16)	0.0149 (13)	−0.0031 (11)	0.0079 (11)	−0.0013 (11)
C16B	0.055 (2)	0.0337 (15)	0.0268 (15)	0.0103 (14)	0.0247 (14)	0.0053 (12)
C17B	0.0357 (15)	0.0207 (12)	0.0317 (14)	0.0012 (10)	0.0154 (12)	−0.0026 (10)
C18B	0.0203 (14)	0.0291 (15)	0.0301 (17)	0.0041 (11)	0.0080 (12)	−0.0032 (12)
C19B	0.0318 (17)	0.0246 (15)	0.0190 (14)	0.0056 (12)	0.0009 (12)	0.0025 (11)
O1C	0.0227 (11)	0.0403 (13)	0.0203 (10)	0.0104 (9)	0.0036 (8)	0.0026 (9)
O2C	0.0235 (11)	0.0226 (10)	0.0182 (10)	0.0063 (8)	0.0076 (8)	−0.0029 (8)
O3C	0.0222 (11)	0.0247 (11)	0.0150 (10)	0.0053 (8)	0.0046 (8)	0.0007 (8)
N1C	0.0208 (14)	0.0303 (15)	0.0171 (13)	−0.0012 (11)	0.0055 (11)	−0.0025 (10)
C1C	0.0211 (12)	0.0216 (11)	0.0135 (11)	−0.0020 (9)	0.0010 (9)	0.0014 (8)
C2C	0.0149 (11)	0.0240 (12)	0.0215 (12)	−0.0005 (9)	0.0016 (9)	0.0019 (9)
C3C	0.0227 (15)	0.0166 (14)	0.0156 (14)	−0.0034 (10)	0.0060 (12)	−0.0009 (10)
C4C	0.0169 (11)	0.0212 (11)	0.0152 (11)	−0.0010 (8)	0.0006 (9)	−0.0001 (8)
C5C	0.0167 (11)	0.0210 (11)	0.0175 (11)	−0.0010 (9)	0.0021 (9)	−0.0016 (9)
C6C	0.0195 (13)	0.0190 (13)	0.0139 (12)	−0.0010 (10)	0.0026 (10)	0.0016 (10)
C7C	0.0204 (13)	0.0196 (14)	0.0192 (13)	−0.0012 (10)	0.0061 (10)	0.0007 (10)
C8C	0.0205 (14)	0.0187 (13)	0.0179 (13)	−0.0005 (10)	0.0040 (11)	0.0001 (10)
C9C	0.0221 (15)	0.0228 (14)	0.0179 (14)	−0.0012 (11)	0.0061 (12)	0.0030 (11)
C10C	0.0169 (13)	0.0164 (13)	0.0165 (14)	−0.0007 (10)	0.0077 (11)	0.0007 (10)
C11C	0.0167 (14)	0.0174 (13)	0.0214 (15)	0.0001 (10)	0.0073 (12)	0.0010 (11)
C12C	0.0175 (13)	0.0166 (13)	0.0175 (13)	0.0006 (10)	0.0093 (11)	−0.0018 (10)
C13C	0.0155 (13)	0.0174 (13)	0.0181 (14)	−0.0014 (10)	0.0036 (11)	0.0009 (11)
C14C	0.0161 (13)	0.0185 (14)	0.0178 (14)	0.0015 (10)	0.0042 (11)	0.0025 (11)
C15C	0.0185 (14)	0.0156 (14)	0.0218 (15)	0.0024 (10)	0.0096 (11)	−0.0015 (11)
C16C	0.0272 (13)	0.0307 (14)	0.0177 (12)	−0.0007 (10)	0.0074 (10)	−0.0032 (10)
C17C	0.0226 (14)	0.063 (2)	0.0263 (15)	0.0053 (13)	0.0086 (12)	−0.0051 (14)
C18C	0.0228 (14)	0.0274 (15)	0.0324 (16)	0.0073 (12)	0.0114 (12)	−0.0032 (12)
C19C	0.0260 (16)	0.0253 (15)	0.0210 (15)	0.0057 (11)	0.0009 (12)	0.0004 (11)
O1D	0.0256 (11)	0.0455 (14)	0.0199 (10)	0.0069 (10)	0.0052 (9)	0.0011 (9)
O2D	0.0234 (10)	0.0205 (10)	0.0175 (10)	0.0048 (8)	0.0057 (8)	−0.0028 (8)
O3D	0.0271 (12)	0.0246 (10)	0.0141 (10)	0.0045 (8)	0.0020 (8)	0.0002 (8)
N1D	0.0310 (15)	0.0231 (14)	0.0195 (13)	0.0009 (11)	0.0127 (11)	0.0004 (10)
C1D	0.0169 (11)	0.0232 (12)	0.0152 (11)	−0.0025 (9)	0.0005 (9)	0.0038 (9)
C2D	0.0159 (11)	0.0189 (11)	0.0198 (12)	−0.0014 (8)	0.0020 (9)	0.0020 (9)

C3D	0.0205 (14)	0.0195 (15)	0.0164 (14)	−0.0033 (11)	0.0060 (11)	−0.0004 (10)
C4D	0.0380 (15)	0.0234 (12)	0.0219 (12)	0.0054 (10)	0.0140 (12)	0.0057 (10)
C5D	0.0360 (14)	0.0180 (11)	0.0243 (12)	0.0009 (10)	0.0142 (11)	0.0028 (9)
C6D	0.0174 (13)	0.0260 (14)	0.0131 (13)	−0.0033 (10)	0.0020 (10)	−0.0019 (10)
C7D	0.0194 (13)	0.0245 (14)	0.0202 (13)	−0.0042 (10)	0.0060 (10)	−0.0008 (10)
C8D	0.0221 (15)	0.0231 (13)	0.0174 (13)	−0.0024 (11)	0.0040 (11)	−0.0016 (10)
C9D	0.0178 (14)	0.0261 (16)	0.0174 (14)	−0.0036 (11)	0.0060 (11)	0.0002 (11)
C10D	0.0176 (14)	0.0184 (13)	0.0132 (13)	−0.0026 (11)	0.0061 (11)	−0.0006 (10)
C11D	0.0141 (13)	0.0192 (13)	0.0204 (15)	0.0000 (10)	0.0060 (11)	0.0022 (11)
C12D	0.0175 (13)	0.0171 (12)	0.0140 (13)	−0.0012 (10)	0.0069 (10)	0.0000 (10)
C13D	0.0176 (14)	0.0203 (14)	0.0190 (15)	−0.0029 (11)	0.0040 (11)	0.0003 (11)
C14D	0.0197 (14)	0.0209 (15)	0.0169 (14)	0.0018 (11)	0.0060 (11)	0.0041 (11)
C15D	0.0219 (15)	0.0175 (15)	0.0220 (15)	−0.0006 (11)	0.0070 (12)	−0.0010 (12)
C16D	0.052 (2)	0.0348 (16)	0.0266 (15)	0.0104 (14)	0.0212 (14)	0.0055 (12)
C17D	0.0370 (15)	0.0242 (13)	0.0300 (14)	−0.0004 (11)	0.0160 (12)	−0.0025 (11)
C18D	0.0223 (14)	0.0219 (14)	0.0249 (14)	0.0050 (10)	0.0076 (11)	−0.0021 (11)
C19D	0.0251 (16)	0.0268 (15)	0.0222 (15)	0.0028 (12)	−0.0018 (12)	0.0011 (12)

Geometric parameters (Å, °)

O1A—C9A	1.240 (4)	O1C—C9C	1.223 (4)
O2A—C12A	1.344 (4)	O2C—C12C	1.384 (4)
O2A—C18A	1.424 (4)	O2C—C18C	1.429 (4)
O3A—C13A	1.360 (4)	O3C—C13C	1.369 (4)
O3A—C19A	1.431 (4)	O3C—C19C	1.431 (4)
N1A—C3A	1.360 (5)	N1C—C3C	1.369 (5)
N1A—C17A	1.442 (4)	N1C—C17C	1.446 (5)
N1A—C16A	1.463 (4)	N1C—C16C	1.453 (4)
C1A—C2A	1.384 (3)	C1C—C2C	1.379 (4)
C1A—C6A	1.400 (4)	C1C—C6C	1.413 (4)
C1A—H1A	0.9300	C1C—H1C	0.9300
C2A—C3A	1.424 (4)	C2C—C3C	1.423 (4)
C2A—H2A	0.9300	C2C—H2C	0.9300
C3A—C4A	1.407 (5)	C3C—C4C	1.412 (5)
C4A—C5A	1.383 (3)	C4C—C5C	1.370 (3)
C4A—H4A	0.9300	C4C—H4C	0.9300
C5A—C6A	1.402 (4)	C5C—C6C	1.406 (4)
C5A—H5A	0.9300	C5C—H5C	0.9300
C6A—C7A	1.454 (5)	C6C—C7C	1.445 (5)
C7A—C8A	1.341 (4)	C7C—C8C	1.345 (4)
C7A—H7A	0.9300	C7C—H7C	0.9300
C8A—C9A	1.472 (5)	C8C—C9C	1.471 (5)
C8A—H8A	0.9300	C8C—H8C	0.9300
C9A—C10A	1.500 (5)	C9C—C10C	1.493 (5)
C10A—C15A	1.372 (5)	C10C—C15C	1.401 (5)
C10A—C11A	1.398 (5)	C10C—C11C	1.418 (5)
C11A—C12A	1.391 (5)	C11C—C12C	1.369 (5)
C11A—H11A	0.9300	C11C—H11C	0.9300
C12A—C13A	1.419 (5)	C12C—C13C	1.421 (5)

C13A—C14A	1.400 (5)	C13C—C14C	1.361 (5)
C14A—C15A	1.383 (5)	C14C—C15C	1.408 (5)
C14A—H14A	0.9300	C14C—H14C	0.9300
C15A—H15A	0.9300	C15C—H15C	0.9300
C16A—H16A	0.9600	C16C—H16G	0.9600
C16A—H16B	0.9600	C16C—H16H	0.9600
C16A—H16C	0.9600	C16C—H16I	0.9600
C17A—H17A	0.9600	C17C—H17G	0.9600
C17A—H17B	0.9600	C17C—H17H	0.9600
C17A—H17C	0.9600	C17C—H17I	0.9600
C18A—H18A	0.9600	C18C—H18G	0.9600
C18A—H18B	0.9600	C18C—H18H	0.9600
C18A—H18C	0.9600	C18C—H18I	0.9600
C19A—H19A	0.9600	C19C—H19G	0.9600
C19A—H19B	0.9600	C19C—H19H	0.9600
C19A—H19C	0.9600	C19C—H19I	0.9600
O1B—C9B	1.238 (5)	O1D—C9D	1.216 (5)
O2B—C12B	1.344 (4)	O2D—C12D	1.379 (4)
O2B—C18B	1.431 (4)	O2D—C18D	1.432 (4)
O3B—C13B	1.362 (4)	O3D—C13D	1.363 (4)
O3B—C19B	1.434 (4)	O3D—C19D	1.423 (4)
N1B—C3B	1.372 (5)	N1D—C3D	1.385 (5)
N1B—C16B	1.453 (4)	N1D—C17D	1.442 (4)
N1B—C17B	1.463 (4)	N1D—C16D	1.458 (4)
C1B—C2B	1.383 (4)	C1D—C2D	1.384 (4)
C1B—C6B	1.402 (4)	C1D—C6D	1.395 (4)
C1B—H1B	0.9300	C1D—H1D	0.9300
C2B—C3B	1.418 (4)	C2D—C3D	1.405 (4)
C2B—H2B	0.9300	C2D—H2D	0.9300
C3B—C4B	1.407 (4)	C3D—C4D	1.414 (4)
C4B—C5B	1.382 (4)	C4D—C5D	1.379 (4)
C4B—H4B	0.9300	C4D—H4D	0.9300
C5B—C6B	1.396 (4)	C5D—C6D	1.399 (4)
C5B—H5B	0.9300	C5D—H5D	0.9300
C6B—C7B	1.460 (5)	C6D—C7D	1.449 (5)
C7B—C8B	1.339 (5)	C7D—C8D	1.348 (5)
C7B—H7B	0.9300	C7D—H7D	0.9300
C8B—C9B	1.475 (5)	C8D—C9D	1.473 (5)
C8B—H8B	0.9300	C8D—H8D	0.9300
C9B—C10B	1.503 (5)	C9D—C10D	1.493 (5)
C10B—C15B	1.377 (5)	C10D—C15D	1.399 (5)
C10B—C11B	1.391 (5)	C10D—C11D	1.418 (5)
C11B—C12B	1.394 (5)	C11D—C12D	1.369 (5)
C11B—H11B	0.9300	C11D—H11D	0.9300
C12B—C13B	1.406 (5)	C12D—C13D	1.414 (5)
C13B—C14B	1.407 (5)	C13D—C14D	1.370 (5)
C14B—C15B	1.383 (5)	C14D—C15D	1.412 (5)
C14B—H14B	0.9300	C14D—H14D	0.9300
C15B—H15B	0.9300	C15D—H15D	0.9300

C16B—H16D	0.9600	C16D—H16J	0.9600
C16B—H16E	0.9600	C16D—H16K	0.9600
C16B—H16F	0.9600	C16D—H16L	0.9600
C17B—H17D	0.9600	C17D—H17J	0.9600
C17B—H17E	0.9600	C17D—H17K	0.9600
C17B—H17F	0.9600	C17D—H17L	0.9600
C18B—H18D	0.9600	C18D—H18J	0.9600
C18B—H18E	0.9600	C18D—H18K	0.9600
C18B—H18F	0.9600	C18D—H18L	0.9600
C19B—H19D	0.9600	C19D—H19J	0.9600
C19B—H19E	0.9600	C19D—H19K	0.9600
C19B—H19F	0.9600	C19D—H19L	0.9600
C12A—O2A—C18A	117.1 (3)	C12C—O2C—C18C	116.1 (3)
C13A—O3A—C19A	116.6 (3)	C13C—O3C—C19C	116.3 (3)
C3A—N1A—C17A	120.8 (3)	C3C—N1C—C17C	120.5 (3)
C3A—N1A—C16A	119.9 (3)	C3C—N1C—C16C	120.7 (3)
C17A—N1A—C16A	119.0 (3)	C17C—N1C—C16C	118.7 (3)
C2A—C1A—C6A	122.1 (2)	C2C—C1C—C6C	122.0 (2)
C2A—C1A—H1A	119.0	C2C—C1C—H1C	119.0
C6A—C1A—H1A	119.0	C6C—C1C—H1C	119.0
C1A—C2A—C3A	120.5 (3)	C1C—C2C—C3C	120.7 (3)
C1A—C2A—H2A	119.8	C1C—C2C—H2C	119.6
C3A—C2A—H2A	119.8	C3C—C2C—H2C	119.6
N1A—C3A—C4A	121.4 (3)	N1C—C3C—C4C	121.1 (3)
N1A—C3A—C2A	121.2 (3)	N1C—C3C—C2C	121.5 (3)
C4A—C3A—C2A	117.4 (3)	C4C—C3C—C2C	117.4 (3)
C5A—C4A—C3A	121.0 (2)	C5C—C4C—C3C	120.8 (2)
C5A—C4A—H4A	119.5	C5C—C4C—H4C	119.6
C3A—C4A—H4A	119.5	C3C—C4C—H4C	119.6
C4A—C5A—C6A	122.0 (2)	C4C—C5C—C6C	122.8 (3)
C4A—C5A—H5A	119.0	C4C—C5C—H5C	118.6
C6A—C5A—H5A	119.0	C6C—C5C—H5C	118.6
C1A—C6A—C5A	117.1 (3)	C5C—C6C—C1C	116.4 (3)
C1A—C6A—C7A	124.6 (3)	C5C—C6C—C7C	119.4 (3)
C5A—C6A—C7A	118.3 (3)	C1C—C6C—C7C	124.2 (3)
C8A—C7A—C6A	127.8 (3)	C8C—C7C—C6C	128.2 (3)
C8A—C7A—H7A	116.1	C8C—C7C—H7C	115.9
C6A—C7A—H7A	116.1	C6C—C7C—H7C	115.9
C7A—C8A—C9A	120.5 (3)	C7C—C8C—C9C	120.7 (3)
C7A—C8A—H8A	119.8	C7C—C8C—H8C	119.6
C9A—C8A—H8A	119.8	C9C—C8C—H8C	119.6
O1A—C9A—C8A	121.3 (3)	O1C—C9C—C8C	122.3 (3)
O1A—C9A—C10A	119.7 (3)	O1C—C9C—C10C	119.8 (3)
C8A—C9A—C10A	119.0 (3)	C8C—C9C—C10C	117.9 (3)
C15A—C10A—C11A	119.3 (3)	C15C—C10C—C11C	118.7 (3)
C15A—C10A—C9A	123.4 (3)	C15C—C10C—C9C	123.1 (3)
C11A—C10A—C9A	117.3 (3)	C11C—C10C—C9C	118.3 (3)
C12A—C11A—C10A	121.1 (3)	C12C—C11C—C10C	120.5 (3)
C12A—C11A—H11A	119.5	C12C—C11C—H11C	119.8

C10A—C11A—H11A	119.5	C10C—C11C—H11C	119.8
O2A—C12A—C11A	126.1 (3)	C11C—C12C—O2C	125.2 (3)
O2A—C12A—C13A	115.2 (3)	C11C—C12C—C13C	120.3 (3)
C11A—C12A—C13A	118.7 (3)	O2C—C12C—C13C	114.5 (3)
O3A—C13A—C14A	125.5 (3)	C14C—C13C—O3C	124.6 (3)
O3A—C13A—C12A	114.8 (3)	C14C—C13C—C12C	119.8 (3)
C14A—C13A—C12A	119.7 (3)	O3C—C13C—C12C	115.7 (3)
C15A—C14A—C13A	119.6 (3)	C13C—C14C—C15C	120.7 (3)
C15A—C14A—H14A	120.2	C13C—C14C—H14C	119.7
C13A—C14A—H14A	120.2	C15C—C14C—H14C	119.7
C10A—C15A—C14A	121.6 (3)	C10C—C15C—C14C	120.1 (3)
C10A—C15A—H15A	119.2	C10C—C15C—H15C	120.0
C14A—C15A—H15A	119.2	C14C—C15C—H15C	120.0
N1A—C16A—H16A	109.5	N1C—C16C—H16G	109.5
N1A—C16A—H16B	109.5	N1C—C16C—H16H	109.5
H16A—C16A—H16B	109.5	H16G—C16C—H16H	109.5
N1A—C16A—H16C	109.5	N1C—C16C—H16I	109.5
H16A—C16A—H16C	109.5	H16G—C16C—H16I	109.5
H16B—C16A—H16C	109.5	H16H—C16C—H16I	109.5
N1A—C17A—H17A	109.5	N1C—C17C—H17G	109.5
N1A—C17A—H17B	109.5	N1C—C17C—H17H	109.5
H17A—C17A—H17B	109.5	H17G—C17C—H17H	109.5
N1A—C17A—H17C	109.5	N1C—C17C—H17I	109.5
H17A—C17A—H17C	109.5	H17G—C17C—H17I	109.5
H17B—C17A—H17C	109.5	H17H—C17C—H17I	109.5
O2A—C18A—H18A	109.5	O2C—C18C—H18G	109.5
O2A—C18A—H18B	109.5	O2C—C18C—H18H	109.5
H18A—C18A—H18B	109.5	H18G—C18C—H18H	109.5
O2A—C18A—H18C	109.5	O2C—C18C—H18I	109.5
H18A—C18A—H18C	109.5	H18G—C18C—H18I	109.5
H18B—C18A—H18C	109.5	H18H—C18C—H18I	109.5
O3A—C19A—H19A	109.5	O3C—C19C—H19G	109.5
O3A—C19A—H19B	109.5	O3C—C19C—H19H	109.5
H19A—C19A—H19B	109.5	H19G—C19C—H19H	109.5
O3A—C19A—H19C	109.5	O3C—C19C—H19I	109.5
H19A—C19A—H19C	109.5	H19G—C19C—H19I	109.5
H19B—C19A—H19C	109.5	H19H—C19C—H19I	109.5
C12B—O2B—C18B	117.5 (3)	C12D—O2D—C18D	116.1 (3)
C13B—O3B—C19B	117.1 (3)	C13D—O3D—C19D	116.6 (3)
C3B—N1B—C16B	119.2 (3)	C3D—N1D—C17D	120.0 (3)
C3B—N1B—C17B	119.5 (3)	C3D—N1D—C16D	118.9 (3)
C16B—N1B—C17B	115.5 (3)	C17D—N1D—C16D	116.3 (3)
C2B—C1B—C6B	121.9 (2)	C2D—C1D—C6D	121.7 (2)
C2B—C1B—H1B	119.0	C2D—C1D—H1D	119.1
C6B—C1B—H1B	119.0	C6D—C1D—H1D	119.1
C1B—C2B—C3B	120.9 (2)	C1D—C2D—C3D	121.1 (2)
C1B—C2B—H2B	119.6	C1D—C2D—H2D	119.5
C3B—C2B—H2B	119.6	C3D—C2D—H2D	119.5
N1B—C3B—C4B	120.9 (3)	N1D—C3D—C2D	122.2 (3)

N1B—C3B—C2B	122.1 (3)	N1D—C3D—C4D	120.6 (3)
C4B—C3B—C2B	117.0 (3)	C2D—C3D—C4D	117.2 (3)
C5B—C4B—C3B	121.0 (3)	C5D—C4D—C3D	120.9 (3)
C5B—C4B—H4B	119.5	C5D—C4D—H4D	119.6
C3B—C4B—H4B	119.5	C3D—C4D—H4D	119.6
C4B—C5B—C6B	122.3 (3)	C4D—C5D—C6D	121.8 (3)
C4B—C5B—H5B	118.9	C4D—C5D—H5D	119.1
C6B—C5B—H5B	118.9	C6D—C5D—H5D	119.1
C5B—C6B—C1B	116.8 (3)	C1D—C6D—C5D	117.3 (3)
C5B—C6B—C7B	118.6 (3)	C1D—C6D—C7D	124.9 (3)
C1B—C6B—C7B	124.6 (3)	C5D—C6D—C7D	117.9 (3)
C8B—C7B—C6B	128.0 (3)	C8D—C7D—C6D	128.7 (3)
C8B—C7B—H7B	116.0	C8D—C7D—H7D	115.6
C6B—C7B—H7B	116.0	C6D—C7D—H7D	115.6
C7B—C8B—C9B	119.5 (3)	C7D—C8D—C9D	118.8 (3)
C7B—C8B—H8B	120.2	C7D—C8D—H8D	120.6
C9B—C8B—H8B	120.2	C9D—C8D—H8D	120.6
O1B—C9B—C8B	120.8 (3)	O1D—C9D—C8D	121.6 (3)
O1B—C9B—C10B	119.1 (3)	O1D—C9D—C10D	119.4 (3)
C8B—C9B—C10B	120.1 (3)	C8D—C9D—C10D	118.8 (3)
C15B—C10B—C11B	119.3 (3)	C15D—C10D—C11D	118.7 (3)
C15B—C10B—C9B	123.1 (3)	C15D—C10D—C9D	124.5 (3)
C11B—C10B—C9B	117.5 (3)	C11D—C10D—C9D	116.8 (3)
C10B—C11B—C12B	121.3 (3)	C12D—C11D—C10D	120.7 (3)
C10B—C11B—H11B	119.3	C12D—C11D—H11D	119.7
C12B—C11B—H11B	119.3	C10D—C11D—H11D	119.7
O2B—C12B—C11B	125.4 (3)	C11D—C12D—O2D	125.0 (3)
O2B—C12B—C13B	115.8 (3)	C11D—C12D—C13D	120.4 (3)
C11B—C12B—C13B	118.7 (3)	O2D—C12D—C13D	114.6 (3)
O3B—C13B—C12B	115.5 (3)	O3D—C13D—C14D	125.0 (3)
O3B—C13B—C14B	124.7 (3)	O3D—C13D—C12D	115.4 (3)
C12B—C13B—C14B	119.8 (3)	C14D—C13D—C12D	119.6 (3)
C15B—C14B—C13B	119.6 (3)	C13D—C14D—C15D	120.6 (3)
C15B—C14B—H14B	120.2	C13D—C14D—H14D	119.7
C13B—C14B—H14B	120.2	C15D—C14D—H14D	119.7
C10B—C15B—C14B	121.3 (3)	C10D—C15D—C14D	120.0 (3)
C10B—C15B—H15B	119.4	C10D—C15D—H15D	120.0
C14B—C15B—H15B	119.4	C14D—C15D—H15D	120.0
N1B—C16B—H16D	109.5	N1D—C16D—H16J	109.5
N1B—C16B—H16E	109.5	N1D—C16D—H16K	109.5
H16D—C16B—H16E	109.5	H16J—C16D—H16K	109.5
N1B—C16B—H16F	109.5	N1D—C16D—H16L	109.5
H16D—C16B—H16F	109.5	H16J—C16D—H16L	109.5
H16E—C16B—H16F	109.5	H16K—C16D—H16L	109.5
N1B—C17B—H17D	109.5	N1D—C17D—H17J	109.5
N1B—C17B—H17E	109.5	N1D—C17D—H17K	109.5
H17D—C17B—H17E	109.5	H17J—C17D—H17K	109.5
N1B—C17B—H17F	109.5	N1D—C17D—H17L	109.5
H17D—C17B—H17F	109.5	H17J—C17D—H17L	109.5

H17E—C17B—H17F	109.5	H17K—C17D—H17L	109.5
O2B—C18B—H18D	109.5	O2D—C18D—H18J	109.5
O2B—C18B—H18E	109.5	O2D—C18D—H18K	109.5
H18D—C18B—H18E	109.5	H18J—C18D—H18K	109.5
O2B—C18B—H18F	109.5	O2D—C18D—H18L	109.5
H18D—C18B—H18F	109.5	H18J—C18D—H18L	109.5
H18E—C18B—H18F	109.5	H18K—C18D—H18L	109.5
O3B—C19B—H19D	109.5	O3D—C19D—H19J	109.5
O3B—C19B—H19E	109.5	O3D—C19D—H19K	109.5
H19D—C19B—H19E	109.5	H19J—C19D—H19K	109.5
O3B—C19B—H19F	109.5	O3D—C19D—H19L	109.5
H19D—C19B—H19F	109.5	H19J—C19D—H19L	109.5
H19E—C19B—H19F	109.5	H19K—C19D—H19L	109.5
C6A—C1A—C2A—C3A	−0.3 (4)	C6C—C1C—C2C—C3C	0.4 (4)
C17A—N1A—C3A—C4A	175.8 (3)	C17C—N1C—C3C—C4C	−178.1 (3)
C16A—N1A—C3A—C4A	1.2 (5)	C16C—N1C—C3C—C4C	−0.4 (5)
C17A—N1A—C3A—C2A	−4.5 (5)	C17C—N1C—C3C—C2C	3.0 (5)
C16A—N1A—C3A—C2A	−179.1 (3)	C16C—N1C—C3C—C2C	−179.3 (3)
C1A—C2A—C3A—N1A	−179.0 (3)	C1C—C2C—C3C—N1C	179.3 (3)
C1A—C2A—C3A—C4A	0.6 (4)	C1C—C2C—C3C—C4C	0.4 (4)
N1A—C3A—C4A—C5A	178.9 (3)	N1C—C3C—C4C—C5C	−179.7 (3)
C2A—C3A—C4A—C5A	−0.8 (4)	C2C—C3C—C4C—C5C	−0.7 (4)
C3A—C4A—C5A—C6A	0.7 (4)	C3C—C4C—C5C—C6C	0.3 (4)
C2A—C1A—C6A—C5A	0.2 (4)	C4C—C5C—C6C—C1C	0.5 (4)
C2A—C1A—C6A—C7A	178.7 (3)	C4C—C5C—C6C—C7C	177.6 (3)
C4A—C5A—C6A—C1A	−0.4 (4)	C2C—C1C—C6C—C5C	−0.8 (4)
C4A—C5A—C6A—C7A	−179.0 (3)	C2C—C1C—C6C—C7C	−177.7 (3)
C1A—C6A—C7A—C8A	9.0 (5)	C5C—C6C—C7C—C8C	173.1 (3)
C5A—C6A—C7A—C8A	−172.5 (3)	C1C—C6C—C7C—C8C	−10.1 (5)
C6A—C7A—C8A—C9A	−173.6 (3)	C6C—C7C—C8C—C9C	174.8 (3)
C7A—C8A—C9A—O1A	4.4 (5)	C7C—C8C—C9C—O1C	−7.3 (5)
C7A—C8A—C9A—C10A	−177.3 (3)	C7C—C8C—C9C—C10C	176.7 (3)
O1A—C9A—C10A—C15A	−164.2 (4)	O1C—C9C—C10C—C15C	165.8 (4)
C8A—C9A—C10A—C15A	17.5 (5)	C8C—C9C—C10C—C15C	−18.1 (5)
O1A—C9A—C10A—C11A	16.5 (5)	O1C—C9C—C10C—C11C	−12.4 (5)
C8A—C9A—C10A—C11A	−161.8 (3)	C8C—C9C—C10C—C11C	163.7 (3)
C15A—C10A—C11A—C12A	0.6 (5)	C15C—C10C—C11C—C12C	2.1 (5)
C9A—C10A—C11A—C12A	180.0 (3)	C9C—C10C—C11C—C12C	−179.6 (3)
C18A—O2A—C12A—C11A	−9.5 (5)	C10C—C11C—C12C—O2C	179.8 (3)
C18A—O2A—C12A—C13A	171.5 (3)	C10C—C11C—C12C—C13C	−1.5 (5)
C10A—C11A—C12A—O2A	−179.0 (3)	C18C—O2C—C12C—C11C	10.1 (5)
C10A—C11A—C12A—C13A	0.0 (5)	C18C—O2C—C12C—C13C	−168.6 (3)
C19A—O3A—C13A—C14A	5.9 (5)	C19C—O3C—C13C—C14C	−10.3 (5)
C19A—O3A—C13A—C12A	−172.3 (3)	C19C—O3C—C13C—C12C	169.7 (3)
O2A—C12A—C13A—O3A	−2.7 (4)	C11C—C12C—C13C—C14C	0.3 (5)
C11A—C12A—C13A—O3A	178.2 (3)	O2C—C12C—C13C—C14C	179.1 (3)
O2A—C12A—C13A—C14A	178.9 (3)	C11C—C12C—C13C—O3C	−179.7 (3)
C11A—C12A—C13A—C14A	−0.2 (5)	O2C—C12C—C13C—O3C	−0.9 (4)
O3A—C13A—C14A—C15A	−178.5 (3)	O3C—C13C—C14C—C15C	−179.8 (3)

C12A—C13A—C14A—C15A	−0.3 (5)	C12C—C13C—C14C—C15C	0.2 (5)
C11A—C10A—C15A—C14A	−1.2 (5)	C11C—C10C—C15C—C14C	−1.6 (5)
C9A—C10A—C15A—C14A	179.5 (3)	C9C—C10C—C15C—C14C	−179.7 (3)
C13A—C14A—C15A—C10A	1.0 (5)	C13C—C14C—C15C—C10C	0.4 (5)
C6B—C1B—C2B—C3B	−1.1 (4)	C6D—C1D—C2D—C3D	1.1 (4)
C16B—N1B—C3B—C4B	12.9 (5)	C17D—N1D—C3D—C2D	15.0 (5)
C17B—N1B—C3B—C4B	165.1 (3)	C16D—N1D—C3D—C2D	169.4 (3)
C16B—N1B—C3B—C2B	−168.6 (3)	C17D—N1D—C3D—C4D	−166.1 (3)
C17B—N1B—C3B—C2B	−16.4 (5)	C16D—N1D—C3D—C4D	−11.7 (5)
C1B—C2B—C3B—N1B	−175.2 (3)	C1D—C2D—C3D—N1D	176.2 (3)
C1B—C2B—C3B—C4B	3.4 (4)	C1D—C2D—C3D—C4D	−2.7 (4)
N1B—C3B—C4B—C5B	175.8 (3)	N1D—C3D—C4D—C5D	−176.8 (3)
C2B—C3B—C4B—C5B	−2.8 (5)	C2D—C3D—C4D—C5D	2.2 (5)
C3B—C4B—C5B—C6B	−0.1 (5)	C3D—C4D—C5D—C6D	0.0 (5)
C4B—C5B—C6B—C1B	2.5 (4)	C2D—C1D—C6D—C5D	1.1 (4)
C4B—C5B—C6B—C7B	−178.0 (3)	C2D—C1D—C6D—C7D	−179.2 (3)
C2B—C1B—C6B—C5B	−1.8 (4)	C4D—C5D—C6D—C1D	−1.6 (5)
C2B—C1B—C6B—C7B	178.7 (3)	C4D—C5D—C6D—C7D	178.6 (3)
C5B—C6B—C7B—C8B	167.0 (3)	C1D—C6D—C7D—C8D	14.2 (6)
C1B—C6B—C7B—C8B	−13.6 (5)	C5D—C6D—C7D—C8D	−166.0 (3)
C6B—C7B—C8B—C9B	−174.3 (3)	C6D—C7D—C8D—C9D	176.3 (3)
C7B—C8B—C9B—O1B	−24.2 (5)	C7D—C8D—C9D—O1D	21.9 (5)
C7B—C8B—C9B—C10B	153.4 (3)	C7D—C8D—C9D—C10D	−153.4 (3)
O1B—C9B—C10B—C15B	−179.9 (3)	O1D—C9D—C10D—C15D	177.9 (4)
C8B—C9B—C10B—C15B	2.6 (5)	C8D—C9D—C10D—C15D	−6.7 (5)
O1B—C9B—C10B—C11B	4.1 (5)	O1D—C9D—C10D—C11D	−3.0 (5)
C8B—C9B—C10B—C11B	−173.5 (3)	C8D—C9D—C10D—C11D	172.4 (3)
C15B—C10B—C11B—C12B	1.5 (5)	C15D—C10D—C11D—C12D	1.1 (5)
C9B—C10B—C11B—C12B	177.7 (3)	C9D—C10D—C11D—C12D	−178.1 (3)
C18B—O2B—C12B—C11B	−13.1 (5)	C10D—C11D—C12D—O2D	179.6 (3)
C18B—O2B—C12B—C13B	167.6 (3)	C10D—C11D—C12D—C13D	−2.0 (5)
C10B—C11B—C12B—O2B	179.0 (3)	C18D—O2D—C12D—C11D	9.4 (5)
C10B—C11B—C12B—C13B	−1.7 (5)	C18D—O2D—C12D—C13D	−169.1 (3)
C19B—O3B—C13B—C12B	−171.2 (3)	C19D—O3D—C13D—C14D	−7.3 (5)
C19B—O3B—C13B—C14B	7.9 (5)	C19D—O3D—C13D—C12D	173.7 (3)
O2B—C12B—C13B—O3B	−0.2 (4)	C11D—C12D—C13D—O3D	−178.4 (3)
C11B—C12B—C13B—O3B	−179.6 (3)	O2D—C12D—C13D—O3D	0.1 (4)
O2B—C12B—C13B—C14B	−179.4 (3)	C11D—C12D—C13D—C14D	2.5 (5)
C11B—C12B—C13B—C14B	1.3 (5)	O2D—C12D—C13D—C14D	−178.9 (3)
O3B—C13B—C14B—C15B	−179.7 (3)	O3D—C13D—C14D—C15D	178.9 (3)
C12B—C13B—C14B—C15B	−0.7 (5)	C12D—C13D—C14D—C15D	−2.1 (5)
C11B—C10B—C15B—C14B	−0.9 (5)	C11D—C10D—C15D—C14D	−0.6 (5)
C9B—C10B—C15B—C14B	−176.9 (3)	C9D—C10D—C15D—C14D	178.5 (3)
C13B—C14B—C15B—C10B	0.5 (5)	C13D—C14D—C15D—C10D	1.2 (5)

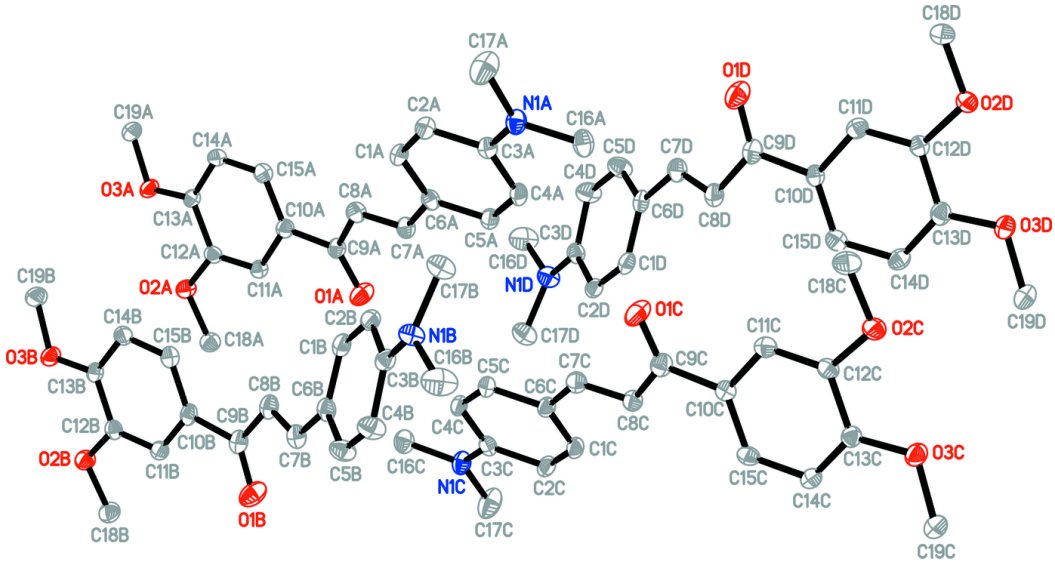
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16C—H16I···O2D^{i}	0.96	2.40	3.306 (4)	157

C16D—H16K···O1B^{ii}	0.96	2.60	3.489 (5)	154
C16D—H16L···O2C^{i}	0.96	2.57	3.460 (4)	155
C18B—H18D···O1C^{iii}	0.96	2.58	3.283 (5)	130
C18C—H18G···O1A^{iv}	0.96	2.56	3.320 (5)	136
C19A—H19B···O2B^{ii}	0.96	2.60	3.446 (5)	147
C2B—H2B···Cg1	0.93	2.92	3.737 (3)	148
C2D—H2D···Cg3	0.93	2.91	3.718 (2)	147
C5A—H5A···Cg4	0.93	2.91	3.559 (3)	128
C5B—H5B···Cg1^{v}	0.93	2.72	3.466 (3)	138
C5C—H5C···Cg2	0.93	2.92	3.559 (3)	128
C5D—H5D···Cg3^{ii}	0.93	2.73	3.481 (3)	139
C14A—H14A···Cg7^{vi}	0.93	3.03	3.742 (4)	135
C14B—H14B···Cg8^{vi}	0.93	3.05	3.773 (4)	136
C14C—H14C···Cg6^{vii}	0.93	2.96	3.676 (4)	135
C14D—H14D···Cg5^{viii}	0.93	3.17	3.875 (4)	134
C18A—H18B···Cg6	0.96	2.67	3.480 (4)	142
C18B—H18E···Cg5^{v}	0.96	2.83	3.683 (4)	149
C18C—H18I···Cg8	0.96	2.82	3.639 (4)	144
C18D—H18L···Cg7^{ii}	0.96	2.70	3.505 (4)	142

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

Fig. 1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N1A
O2D
C19A
C2A
C11D
C16A
C14A
C1A
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C7D
C12D
C15A
C4D
C9D
O3A
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C4A
C10D
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C10A
C6A
C6D
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C11B
C5B
C16C
C3C
C15C
C2C
N1C
C14C
C18B
O1B
C17C
C19C

Fig. 2