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10-Methoxy-5*H*-dibenz[*b*,*f*]azepine

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.055
wR factor = 0.146
Data-to-parameter ratio = 9.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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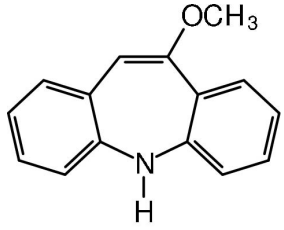
The structure of the title compound, $C_{15}H_{13}NO$, has six independent molecules in the asymmetric unit; in each case, the seven-membered ring adopts a boat conformation and the overall molecular shape is that of a butterfly. All molecules display N—H···C=C close contacts, instead of N—H···O interactions. The intramolecular dihedral angles between the benzene rings are within the range 43.7 (1)–46.4 (1)° for the six molecules.

Comment

The title compound, (I), is used as an intermediate for the synthesis of the registered anticonvulsant drug oxcarbazepine (Kricka & Ledwith, 1974), the structure of which has recently been reported (Hempel *et al.*, 2005). As part of a series of studies into the structural aspects of iminostilbene analogues, the structure of (I) was determined and is reported here.



(I)

A search of the Cambridge Structural Database (CSD, Version 5.26; Allen, 2002) reveals 29 compounds that contain a dibenz[*b*,*f*]azepine moiety, with all bar four being either structures or adducts of 5*H*-dibenz[*b*,*f*]azepine-5-carboxamide (carbamazepine). The structure of (I) has six unique molecules in the asymmetric unit (Fig. 1); in each case, the seven-membered ring adopts a boat conformation (Cremer & Pople, 1975) and the overall molecular shape is that of a butterfly. The intramolecular dihedral angles between the benzene rings are 43.7 (1), 45.1 (1), 46.4 (1), 44.7 (1), 44.7 (1) and 45.2 (1)° for molecules *A* to *F*, respectively. All molecules display N—H···C=C close contacts, listed in Table 1, instead of N—H···O interactions. These close contacts all occur between equivalent molecules in the *b*-cell direction. The unit-cell packing of (I) is shown in Fig. 2.

Experimental

The title compound was prepared by brominating *N*-acetyl-5*H*-dibenz[*b*,*f*]azepine (2.35 g, 10 mmol) using bromine (3.2 g, 20 mmol)

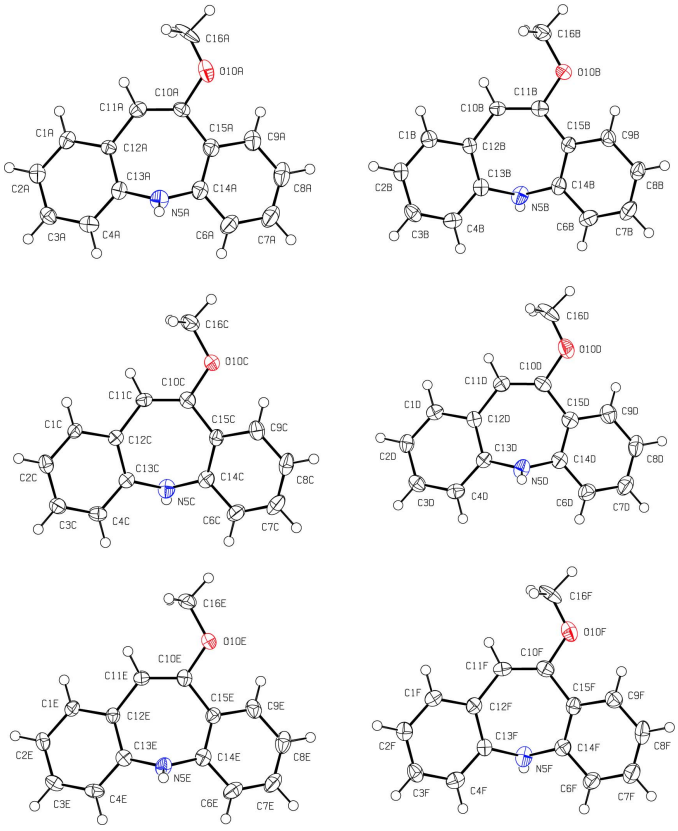


Figure 1
The molecular configuration and atom-numbering scheme for the six molecules in the asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radius. All molecules have been separately plotted in comparable orientations.

in dichloromethane (5 ml) to obtain the dibromo derivative, which was further refluxed with KOH (1.12 g, 20 mmol) in CH_3OH (5 ml) to yield the product. Crystals were grown from a dichloromethane–ethanol (1:1 *v*/*v*) solution.

Crystal data

$C_{15}H_{13}NO$
M_r = 223.26
Monoclinic, *C*2
a = 54.925 (11) Å
b = 5.8189 (12) Å
c = 21.628 (4) Å
β = 98.14 (3)°
V = 6843 (2) Å^3
Z = 24
D_x = 1.300 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 7575 reflections
θ = 2.9–27.5°
μ = 0.08 mm^{-1}
T = 120 (2) K
Prism, yellow
0.38 × 0.34 × 0.14 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.970, T_{max} = 0.989
38719 measured reflections
8443 independent reflections
5366 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.5°
h = −70 → 69
k = −7 → 7
l = −26 → 28

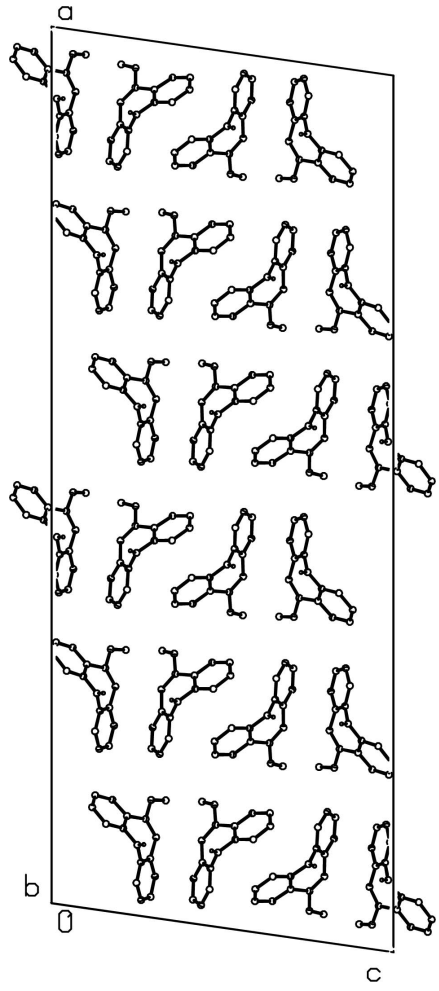


Figure 2
The unit cell contents of (I), viewed down the *b* cell axis. All atoms are drawn as circles of arbitrary radii. For clarity, all H atoms except those of the NH groups have been omitted.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.146
S = 1.18
8443 reflections
926 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0014 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5*A*—H5*A*···C11*A*^{i}	0.88	2.54	3.407 (5)	167
N5*B*—H5*B*···C11*B*^{i}	0.88	2.52	3.388 (5)	167
N5*C*—H5*C*···C11*C*^{i}	0.88	2.54	3.403 (5)	167
N5*D*—H5*D*···C11*D*^{i}	0.88	2.53	3.388 (5)	166
N5*E*—H5*E*···C11*E*^{i}	0.88	2.54	3.405 (5)	167
N5*F*—H5*F*···C11*F*^{i}	0.88	2.53	3.391 (5)	167

Symmetry code: (i) $x, 1 + y, z$.

All H atoms were included in the refinement in calculated positions, in the riding-model approximation, with C—H distances of 0.95

(ArH) and 0.98 Å (CH_3) and an N—H distance of 0.88 Å. The isotropic displacement parameters for all H atoms were set equal to $1.25U_{eq}$ of the carrier atom. In the absence of significant anomalous scattering, 6006 measured Friedel pairs were merged.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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supporting information

Acta Cryst. (2005). E**61**, o1757–o1759 [https://doi.org/10.1107/S1600536805015059]

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$V = 6843$ (2) Å^3
$Z = 24$
$F(000) = 2832$
$D_x = 1.300$ Mg m^{-3}
Melting point: 397 K
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Cell parameters from 7575 reflections
$\theta = 2.9$–27.5°
$\mu = 0.08$ mm^{-1}
$T = 120$ K
Prism, yellow
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Data collection

Nonius KappaCCD diffractometer
Radiation source: Bruker Nonius FR591 rotating anode
10 cm confocal mirrors monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
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$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -70 \rightarrow 69$
$k = -7 \rightarrow 7$
$l = -26 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.146$
$S = 1.18$
8443 reflections
926 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0014 (2)

Special details

Experimental. The minimum and maximum absorption values stated above are those calculated in *SHELXL97* from the given crystal dimensions. The ratio of minimum to maximum apparent transmission was determined experimentally as 0.857355.

Geometry. Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)
- 9.9097 (0.0670) *x* - 2.4174 (0.0065) *y* + 19.6404 (0.0150) *z* = 1.8276 (0.0170)
* -0.0025 (0.0022) C1A * 0.0002 (0.0022) C2A * 0.0018 (0.0022) C3A * -0.0016 (0.0023) C4A * -0.0006 (0.0022) C13A * 0.0026 (0.0022) C12A
Rms deviation of fitted atoms = 0.0018
39.8004 (0.0583) *x* + 3.2459 (0.0069) *y* - 10.8822 (0.0276) *z* = 9.9792 (0.0237)
Angle to previous plane (with approximate e.s.d.) = 43.68 (0.13)
* -0.0048 (0.0025) C6A * 0.0062 (0.0027) C7A * -0.0002 (0.0027) C8A * -0.0070 (0.0025) C9A * 0.0082 (0.0024) C15A * -0.0024 (0.0024) C14A
Rms deviation of fitted atoms = 0.0055
- 4.3373 (0.0689) *x* + 2.4639 (0.0066) *y* + 19.5639 (0.0152) *z* = 3.2892 (0.0144)
Angle to previous plane (with approximate e.s.d.) = 79.27 (0.10)
* 0.0096 (0.0022) C1B * 0.0049 (0.0022) C2B * -0.0136 (0.0023) C3B * 0.0076 (0.0023) C4B * 0.0067 (0.0022) C13B * -0.0152 (0.0022) C12B
Rms deviation of fitted atoms = 0.0103
34.3116 (0.0594) *x* + 2.8715 (0.0066) *y* + 11.0439 (0.0249) *z* = 12.1049 (0.0148)
Angle to previous plane (with approximate e.s.d.) = 45.11 (0.12)
* -0.0042 (0.0023) C6B * 0.0124 (0.0024) C7B * -0.0043 (0.0024) C8B * -0.0115 (0.0023) C9B * 0.0194 (0.0022) C15B * -0.0117 (0.0022) C14B
Rms deviation of fitted atoms = 0.0118
- 3.4142 (0.0697) *x* + 2.4203 (0.0063) *y* + 19.6149 (0.0148) *z* = 7.5931 (0.0057)
Angle to previous plane (with approximate e.s.d.) = 44.32 (0.12)
* 0.0045 (0.0021) C1C * 0.0008 (0.0022) C2C * -0.0033 (0.0023) C3C * 0.0002 (0.0023) C4C * 0.0051 (0.0022) C13C * -0.0074 (0.0021) C12C
Rms deviation of fitted atoms = 0.0043
35.0422 (0.0608) *x* + 3.0540 (0.0068) *y* + 10.1102 (0.0265) *z* = 9.1765 (0.0059)
Angle to previous plane (with approximate e.s.d.) = 46.38 (0.12)
* -0.0043 (0.0024) C6C * 0.0097 (0.0025) C7C * -0.0014 (0.0024) C8C * -0.0119 (0.0023) C9C * 0.0169 (0.0022) C15C * -0.0090 (0.0023) C14C
Rms deviation of fitted atoms = 0.0102
- 8.8499 (0.0689) *x* - 2.3763 (0.0063) *y* + 19.7298 (0.0146) *z* = 7.1423 (0.0090)
Angle to previous plane (with approximate e.s.d.) = 79.10 (0.10)
* -0.0078 (0.0022) C1D * 0.0010 (0.0022) C2D * 0.0048 (0.0023) C3D * -0.0036 (0.0023) C4D * -0.0031 (0.0022) C13D * 0.0088 (0.0022) C12D
Rms deviation of fitted atoms = 0.0055
40.0364 (0.0582) *x* + 3.1845 (0.0069) *y* - 11.0375 (0.0274) *z* = 0.4032 (0.0201)
Angle to previous plane (with approximate e.s.d.) = 44.73 (0.13)
* -0.0108 (0.0025) C6D * 0.0104 (0.0026) C7D * -0.0001 (0.0026) C8D * -0.0097 (0.0025) C9D * 0.0092 (0.0023) C15D * 0.0010 (0.0023) C14D
Rms deviation of fitted atoms = 0.0082
-10.5790 (0.0692) *x* + 2.4460 (0.0065) *y* + 19.5737 (0.0150) *z* = 16.7598 (0.0136)
Angle to previous plane (with approximate e.s.d.) = 74.04 (0.10)
* -0.0007 (0.0022) C1E * 0.0041 (0.0022) C2E * -0.0032 (0.0023) C3E * -0.0011 (0.0023) C4E * 0.0044 (0.0022) C13E * -0.0035 (0.0022) C12E
Rms deviation of fitted atoms = 0.0031
- 42.0032 (0.0533) *x* + 2.9678 (0.0068) *y* + 10.7720 (0.0261) *z* = 8.1642 (0.0187)
Angle to previous plane (with approximate e.s.d.) = 44.70 (0.13)
* -0.0081 (0.0024) C6E * 0.0130 (0.0025) C7E * -0.0028 (0.0025) C8E * -0.0118 (0.0023) C9E * 0.0163 (0.0022) C15E * -0.0066 (0.0023) C14E
Rms deviation of fitted atoms = 0.0107
- 4.9888 (0.0691) *x* - 2.3785 (0.0065) *y* + 19.7208 (0.0148) *z* = 17.2986 (0.0176)
Angle to previous plane (with approximate e.s.d.) = 77.38 (0.10)
* -0.0041 (0.0022) C1F * 0.0006 (0.0022) C2F * 0.0036 (0.0023) C3F * -0.0043 (0.0023) C4F * 0.0008 (0.0022) C13F * 0.0034 (0.0021) C12F
Rms deviation of fitted atoms = 0.0032
32.6303 (0.0652) *x* - 3.1884 (0.0068) *y* + 10.7897 (0.0270) *z* = 10.9191 (0.0287)
Angle to previous plane (with approximate e.s.d.) = 45.19 (0.12)
* 0.0059 (0.0024) C6F * -0.0077 (0.0025) C7F * 0.0023 (0.0026) C8F * 0.0048 (0.0024) C9F * -0.0064 (0.0023) C15F * 0.0012 (0.0024) C14F
Rms deviation of fitted atoms = 0.0052

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1A	0.21696 (5)	0.7580 (7)	0.29568 (13)	0.0254 (8)
H1A	0.2202	0.6118	0.2791	0.032*
C2A	0.19278 (6)	0.8303 (7)	0.29253 (14)	0.0282 (9)
H2A	0.1797	0.7345	0.2742	0.035*
C3A	0.18786 (6)	1.0422 (7)	0.31621 (14)	0.0270 (9)
H3A	0.1713	1.0933	0.3143	0.034*
C4A	0.20696 (6)	1.1803 (7)	0.34267 (14)	0.0277 (9)
H4A	0.2035	1.3267	0.3588	0.035*
N5A	0.25045 (5)	1.2626 (6)	0.36875 (12)	0.0298 (7)
H5A	0.2514	1.3980	0.3511	0.037*
C6A	0.27086 (6)	1.3375 (8)	0.47302 (15)	0.0359 (10)
H6A	0.2605	1.4672	0.4745	0.045*
C7A	0.28883 (7)	1.2885 (8)	0.52313 (16)	0.0422 (11)
H7A	0.2909	1.3861	0.5587	0.053*
C8A	0.30371 (7)	1.0980 (9)	0.52130 (16)	0.0418 (11)
H8A	0.3159	1.0639	0.5557	0.052*
C9A	0.30085 (6)	0.9577 (8)	0.46962 (15)	0.0344 (10)
H9A	0.3110	0.8260	0.4690	0.043*
C10A	0.28173 (5)	0.8525 (6)	0.36239 (14)	0.0240 (8)
O10A	0.30468 (4)	0.7506 (5)	0.35871 (11)	0.0378 (7)
C16A	0.30607 (6)	0.5742 (8)	0.32376 (17)	0.0397 (11)
H16A	0.2950	0.4539	0.3351	0.050*
H17A	0.3230	0.5165	0.3295	0.050*
H18A	0.3012	0.6175	0.2800	0.050*
C11A	0.26186 (5)	0.8058 (7)	0.32154 (13)	0.0251 (8)
H11A	0.2642	0.7057	0.2881	0.031*
C12A	0.23660 (5)	0.8925 (6)	0.32241 (13)	0.0210 (8)
C13A	0.23124 (6)	1.1076 (7)	0.34603 (14)	0.0251 (8)
C14A	0.26809 (6)	1.1960 (7)	0.42044 (15)	0.0269 (9)
C15A	0.28315 (6)	1.0054 (7)	0.41769 (15)	0.0271 (8)
C1B	0.21280 (6)	0.2639 (7)	0.18256 (13)	0.0277 (8)
H1B	0.2160	0.1195	0.2025	0.035*
C2B	0.18878 (6)	0.3360 (7)	0.16792 (14)	0.0281 (9)
H2B	0.1757	0.2417	0.1774	0.035*
C3B	0.18389 (6)	0.5468 (7)	0.13934 (15)	0.0301 (9)
H3B	0.1674	0.5962	0.1281	0.038*
C4B	0.20328 (6)	0.6868 (7)	0.12709 (14)	0.0285 (9)
H4B	0.1999	0.8336	0.1086	0.036*
N5B	0.24684 (5)	0.7643 (6)	0.13247 (11)	0.0287 (7)
H5B	0.2482	0.8985	0.1514	0.036*
C6B	0.26751 (6)	0.8472 (7)	0.04431 (15)	0.0326 (9)
H6B	0.2580	0.9836	0.0379	0.041*
C7B	0.28485 (6)	0.7973 (8)	0.00491 (15)	0.0349 (10)
H7B	0.2873	0.9008	−0.0276	0.044*
C8B	0.29834 (6)	0.5984 (8)	0.01319 (15)	0.0304 (9)

H8B	0.3099	0.5628	−0.0141	0.038*
C9B	0.29508 (5)	0.4487 (7)	0.06159 (14)	0.0273 (9)
H9B	0.3043	0.3102	0.0666	0.034*
C10B	0.27702 (6)	0.3480 (6)	0.15718 (14)	0.0251 (8)
O10B	0.29939 (4)	0.2420 (5)	0.17310 (10)	0.0315 (6)
C16B	0.30099 (6)	0.0613 (7)	0.21719 (16)	0.0340 (10)
H16B	0.2984	0.1226	0.2580	0.043*
H17B	0.3173	−0.0098	0.2206	0.043*
H18B	0.2884	−0.0541	0.2036	0.043*
C11B	0.25765 (5)	0.3063 (6)	0.18670 (14)	0.0236 (8)
H11B	0.2603	0.2096	0.2224	0.030*
C12B	0.23252 (5)	0.3967 (6)	0.16894 (13)	0.0211 (8)
C13B	0.22752 (6)	0.6134 (7)	0.14166 (14)	0.0233 (8)
C14B	0.26406 (6)	0.6994 (7)	0.09279 (14)	0.0254 (8)
C15B	0.27823 (5)	0.5004 (7)	0.10330 (14)	0.0230 (8)
C1C	0.04741 (5)	0.7547 (7)	0.30247 (13)	0.0220 (8)
H1C	0.0509	0.6092	0.3216	0.028*
C2C	0.02337 (6)	0.8246 (7)	0.28948 (14)	0.0275 (9)
H2C	0.0105	0.7282	0.2991	0.034*
C3C	0.01816 (6)	1.0387 (7)	0.26194 (14)	0.0285 (9)
H3C	0.0016	1.0891	0.2526	0.036*
C4C	0.03700 (6)	1.1774 (7)	0.24829 (14)	0.0259 (8)
H4C	0.0333	1.3233	0.2296	0.032*
N5C	0.08049 (5)	1.2600 (5)	0.25095 (11)	0.0278 (7)
H5C	0.0820	1.3944	0.2698	0.035*
C6C	0.09938 (6)	1.3360 (7)	0.15920 (15)	0.0350 (10)
H6C	0.0895	1.4701	0.1523	0.044*
C7C	0.11615 (6)	1.2819 (8)	0.11881 (15)	0.0376 (10)
H7C	0.1178	1.3811	0.0848	0.047*
C8C	0.13029 (6)	1.0871 (8)	0.12755 (15)	0.0347 (10)
H8C	0.1416	1.0506	0.0995	0.043*
C9C	0.12801 (5)	0.9431 (7)	0.17790 (14)	0.0294 (9)
H9C	0.1375	0.8064	0.1835	0.037*
C10C	0.11134 (5)	0.8477 (6)	0.27525 (14)	0.0228 (8)
O10C	0.13404 (4)	0.7454 (5)	0.29123 (10)	0.0305 (6)
C16C	0.13586 (6)	0.5623 (7)	0.33392 (16)	0.0334 (9)
H16C	0.1326	0.6185	0.3747	0.042*
H17C	0.1524	0.4966	0.3380	0.042*
H18C	0.1238	0.4439	0.3189	0.042*
C11C	0.09219 (5)	0.8029 (6)	0.30571 (13)	0.0230 (8)
H11C	0.0952	0.7067	0.3415	0.029*
C12C	0.06690 (5)	0.8898 (6)	0.28858 (13)	0.0205 (8)
C13C	0.06134 (6)	1.1066 (6)	0.26151 (14)	0.0227 (8)
C14C	0.09716 (6)	1.1932 (6)	0.20956 (14)	0.0244 (8)
C15C	0.11173 (5)	0.9977 (6)	0.22067 (14)	0.0229 (8)
C1D	0.05119 (6)	0.2552 (7)	0.41531 (13)	0.0261 (8)
H1D	0.0544	0.1096	0.3983	0.033*
C2D	0.02709 (6)	0.3261 (7)	0.41348 (14)	0.0283 (9)

H2D	0.0140	0.2291	0.3961	0.035*
C3D	0.02223 (6)	0.5392 (7)	0.43716 (14)	0.0291 (9)
H3D	0.0057	0.5895	0.4362	0.036*
C4D	0.04164 (6)	0.6801 (7)	0.46241 (14)	0.0278 (9)
H4D	0.0383	0.8272	0.4783	0.035*
N5D	0.08504 (5)	0.7621 (6)	0.48637 (11)	0.0295 (7)
H5D	0.0860	0.8965	0.4682	0.037*
C6D	0.10578 (6)	0.8383 (7)	0.59002 (15)	0.0343 (10)
H6D	0.0953	0.9677	0.5915	0.043*
C7D	0.12365 (6)	0.7933 (8)	0.63993 (16)	0.0388 (10)
H7D	0.1259	0.8936	0.6749	0.048*
C8D	0.13840 (7)	0.6000 (8)	0.63861 (16)	0.0385 (11)
H8D	0.1506	0.5661	0.6731	0.048*
C9D	0.13532 (6)	0.4573 (8)	0.58712 (15)	0.0341 (10)
H9D	0.1453	0.3243	0.5869	0.043*
C10D	0.11616 (6)	0.3505 (7)	0.48011 (14)	0.0264 (8)
O10D	0.13892 (4)	0.2516 (5)	0.47639 (11)	0.0371 (7)
C16D	0.14041 (6)	0.0739 (8)	0.44047 (17)	0.0397 (11)
H16D	0.1288	−0.0445	0.4501	0.050*
H17D	0.1572	0.0122	0.4476	0.050*
H18D	0.1363	0.1201	0.3967	0.050*
C11D	0.09608 (5)	0.3030 (7)	0.43942 (14)	0.0261 (9)
H11D	0.0982	0.2027	0.4059	0.033*
C12D	0.07099 (6)	0.3905 (7)	0.44133 (14)	0.0230 (8)
C13D	0.06581 (6)	0.6074 (6)	0.46452 (14)	0.0235 (8)
C14D	0.10276 (6)	0.6985 (7)	0.53764 (14)	0.0261 (8)
C15D	0.11779 (6)	0.5041 (7)	0.53535 (15)	0.0265 (8)
C1E	0.11982 (5)	0.7562 (7)	0.82646 (13)	0.0239 (8)
H1E	0.1165	0.6100	0.8429	0.030*
C2E	0.14401 (6)	0.8296 (7)	0.83061 (14)	0.0273 (9)
H2E	0.1570	0.7349	0.8499	0.034*
C3E	0.14906 (6)	1.0395 (7)	0.80674 (15)	0.0268 (9)
H3E	0.1656	1.0903	0.8090	0.033*
C4E	0.13001 (6)	1.1772 (7)	0.77935 (15)	0.0277 (9)
H4E	0.1336	1.3228	0.7630	0.035*
N5E	0.08650 (5)	1.2581 (5)	0.75166 (11)	0.0277 (7)
H5E	0.0852	1.3925	0.7695	0.035*
C6E	0.06654 (6)	1.3394 (7)	0.64759 (15)	0.0350 (10)
H6E	0.0764	1.4735	0.6477	0.044*
C7E	0.04933 (6)	1.2894 (8)	0.59624 (16)	0.0374 (10)
H7E	0.0471	1.3918	0.5617	0.047*
C8E	0.03547 (7)	1.0926 (8)	0.59493 (16)	0.0362 (10)
H8E	0.0239	1.0574	0.5592	0.045*
C9E	0.03836 (5)	0.9456 (7)	0.64586 (14)	0.0301 (9)
H9E	0.0289	0.8085	0.6444	0.038*
C10E	0.05588 (5)	0.8430 (6)	0.75470 (14)	0.0231 (8)
O10E	0.03337 (4)	0.7398 (5)	0.75442 (9)	0.0306 (6)
C16E	0.03174 (6)	0.5574 (7)	0.79614 (16)	0.0330 (10)

H16E	0.0441	0.4405	0.7903	0.041*
H17E	0.0153	0.4893	0.7881	0.041*
H18E	0.0347	0.6150	0.8391	0.041*
C11E	0.07507 (5)	0.8017 (6)	0.79825 (13)	0.0231 (8)
H11E	0.0723	0.7060	0.8321	0.029*
C12E	0.10035 (5)	0.8906 (6)	0.79901 (13)	0.0214 (8)
C13E	0.10569 (6)	1.1060 (7)	0.77538 (14)	0.0246 (8)
C14E	0.06944 (6)	1.1939 (7)	0.69912 (14)	0.0256 (8)
C15E	0.05507 (5)	0.9964 (7)	0.69965 (14)	0.0237 (8)
C1F	0.11522 (6)	0.2524 (7)	0.93657 (13)	0.0264 (8)
H1F	0.1120	0.1061	0.9177	0.033*
C2F	0.13941 (6)	0.3251 (7)	0.95169 (14)	0.0291 (9)
H2F	0.1525	0.2288	0.9434	0.036*
C3F	0.14433 (6)	0.5389 (7)	0.97886 (15)	0.0311 (10)
H3F	0.1608	0.5899	0.9896	0.039*
C4F	0.12484 (6)	0.6777 (7)	0.99028 (14)	0.0286 (9)
H4F	0.1281	0.8251	1.0084	0.036*
N5F	0.08139 (5)	0.7597 (5)	0.98453 (11)	0.0294 (7)
H5F	0.0803	0.8948	0.9660	0.037*
C6F	0.06114 (6)	0.8344 (7)	1.07419 (15)	0.0336 (10)
H6F	0.0714	0.9650	1.0828	0.042*
C7F	0.04344 (6)	0.7857 (8)	1.11209 (16)	0.0374 (10)
H7F	0.0414	0.8846	1.1459	0.047*
C8F	0.02876 (7)	0.5937 (8)	1.10067 (16)	0.0395 (11)
H8F	0.0168	0.5586	1.1270	0.049*
C9F	0.03156 (6)	0.4524 (7)	1.05067 (15)	0.0309 (9)
H9F	0.0214	0.3201	1.0431	0.039*
C10F	0.05038 (6)	0.3474 (7)	0.95691 (14)	0.0278 (9)
O10F	0.02768 (4)	0.2466 (5)	0.93739 (10)	0.0365 (7)
C16F	0.02637 (6)	0.0677 (8)	0.90018 (16)	0.0382 (11)
H16F	0.0301	0.1150	0.8591	0.048*
H17F	0.0097	0.0031	0.8958	0.048*
H18F	0.0383	−0.0487	0.9179	0.048*
C11F	0.07041 (5)	0.3018 (6)	0.93010 (13)	0.0246 (8)
H11F	0.0681	0.2013	0.8952	0.031*
C12F	0.09552 (6)	0.3895 (7)	0.94848 (13)	0.0239 (8)
C13F	0.10062 (6)	0.6046 (7)	0.97560 (14)	0.0229 (8)
C14F	0.06399 (6)	0.6936 (7)	1.02355 (15)	0.0258 (8)
C15F	0.04909 (6)	0.5004 (7)	1.01081 (14)	0.0255 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.0287 (18)	0.028 (2)	0.0204 (16)	−0.0053 (18)	0.0051 (13)	0.0011 (17)
C2A	0.0256 (18)	0.036 (3)	0.0229 (17)	−0.0059 (18)	0.0049 (13)	0.0024 (17)
C3A	0.0240 (17)	0.034 (3)	0.0234 (18)	0.0034 (17)	0.0039 (14)	0.0047 (18)
C4A	0.0351 (19)	0.027 (2)	0.0232 (17)	0.0055 (18)	0.0097 (15)	0.0079 (16)
N5A	0.0364 (16)	0.0190 (18)	0.0331 (15)	−0.0042 (15)	0.0024 (12)	0.0071 (15)

C6A	0.0363 (19)	0.038 (3)	0.034 (2)	−0.0101 (19)	0.0087 (16)	−0.013 (2)
C7A	0.041 (2)	0.054 (3)	0.032 (2)	−0.013 (2)	0.0061 (16)	−0.016 (2)
C8A	0.036 (2)	0.061 (3)	0.027 (2)	−0.011 (2)	−0.0009 (17)	−0.001 (2)
C9A	0.0305 (19)	0.041 (3)	0.031 (2)	−0.0029 (19)	0.0007 (15)	0.0005 (19)
C10A	0.0203 (17)	0.022 (2)	0.0304 (18)	0.0017 (16)	0.0065 (14)	0.0012 (16)
O10A	0.0216 (12)	0.049 (2)	0.0412 (14)	−0.0035 (14)	−0.0029 (10)	0.0033 (15)
C16A	0.0217 (18)	0.052 (3)	0.050 (2)	0.020 (2)	0.0202 (17)	0.024 (2)
C11A	0.0284 (17)	0.028 (2)	0.0203 (16)	−0.0017 (17)	0.0087 (13)	−0.0001 (16)
C12A	0.0213 (16)	0.021 (2)	0.0209 (17)	0.0016 (15)	0.0037 (13)	0.0011 (15)
C13A	0.0266 (18)	0.025 (2)	0.0240 (18)	−0.0039 (17)	0.0028 (14)	0.0025 (17)
C14A	0.0255 (17)	0.030 (2)	0.0254 (18)	−0.0074 (17)	0.0062 (14)	0.0003 (17)
C15A	0.0217 (16)	0.034 (2)	0.0267 (18)	−0.0049 (17)	0.0066 (14)	−0.0002 (17)
C1B	0.0290 (18)	0.030 (2)	0.0245 (17)	−0.0001 (18)	0.0045 (14)	−0.0027 (18)
C2B	0.0245 (17)	0.031 (3)	0.0303 (18)	−0.0034 (17)	0.0079 (14)	−0.0022 (18)
C3B	0.0264 (18)	0.037 (3)	0.0270 (19)	0.0071 (18)	0.0050 (15)	−0.0072 (18)
C4B	0.038 (2)	0.026 (2)	0.0221 (17)	0.0055 (18)	0.0034 (15)	−0.0021 (16)
N5B	0.0381 (16)	0.0171 (18)	0.0320 (15)	−0.0041 (15)	0.0089 (12)	−0.0051 (15)
C6B	0.0344 (19)	0.030 (3)	0.0312 (19)	−0.0055 (18)	−0.0035 (15)	0.0073 (18)
C7B	0.035 (2)	0.042 (3)	0.0268 (18)	−0.015 (2)	0.0000 (15)	0.010 (2)
C8B	0.0249 (18)	0.044 (3)	0.0224 (19)	−0.0078 (19)	0.0020 (15)	0.0046 (19)
C9B	0.0198 (16)	0.033 (2)	0.0282 (19)	−0.0039 (17)	0.0022 (14)	0.0003 (17)
C10B	0.0254 (17)	0.024 (2)	0.0243 (17)	−0.0028 (16)	−0.0033 (14)	−0.0028 (16)
O10B	0.0221 (12)	0.0366 (18)	0.0355 (13)	0.0029 (12)	0.0032 (10)	0.0090 (13)
C16B	0.0254 (18)	0.035 (3)	0.040 (2)	0.0013 (18)	−0.0012 (15)	0.003 (2)
C11B	0.0251 (17)	0.023 (2)	0.0220 (16)	0.0028 (16)	0.0007 (13)	0.0012 (16)
C12B	0.0214 (17)	0.022 (2)	0.0198 (17)	−0.0011 (15)	0.0035 (13)	−0.0036 (15)
C13B	0.0259 (17)	0.023 (2)	0.0211 (18)	−0.0030 (16)	0.0034 (14)	−0.0070 (16)
C14B	0.0242 (17)	0.028 (2)	0.0237 (18)	−0.0073 (17)	0.0028 (14)	−0.0036 (17)
C15B	0.0222 (16)	0.025 (2)	0.0218 (17)	−0.0043 (16)	0.0023 (13)	−0.0017 (16)
C1C	0.0232 (16)	0.023 (2)	0.0198 (15)	−0.0011 (16)	0.0040 (12)	0.0032 (16)
C2C	0.0220 (17)	0.037 (3)	0.0237 (17)	−0.0020 (18)	0.0053 (13)	−0.0051 (18)
C3C	0.0257 (18)	0.032 (3)	0.0273 (19)	0.0044 (17)	0.0031 (15)	0.0016 (18)
C4C	0.0305 (18)	0.020 (2)	0.0264 (18)	0.0048 (17)	0.0015 (14)	−0.0021 (16)
N5C	0.0334 (15)	0.0170 (18)	0.0342 (15)	−0.0042 (15)	0.0085 (12)	−0.0052 (15)
C6C	0.0308 (19)	0.037 (3)	0.036 (2)	−0.0062 (19)	−0.0013 (16)	0.013 (2)
C7C	0.039 (2)	0.044 (3)	0.0280 (19)	−0.016 (2)	0.0001 (16)	0.013 (2)
C8C	0.0303 (19)	0.053 (3)	0.0216 (19)	−0.014 (2)	0.0060 (15)	−0.001 (2)
C9C	0.0215 (16)	0.034 (3)	0.0321 (19)	−0.0079 (17)	0.0030 (14)	−0.0046 (18)
C10C	0.0206 (16)	0.022 (2)	0.0251 (17)	−0.0042 (16)	−0.0003 (13)	−0.0042 (16)
O10C	0.0210 (11)	0.0363 (18)	0.0344 (12)	0.0018 (12)	0.0049 (9)	0.0091 (13)
C16C	0.0228 (17)	0.034 (3)	0.042 (2)	0.0017 (17)	−0.0003 (15)	0.004 (2)
C11C	0.0266 (17)	0.022 (2)	0.0192 (15)	0.0033 (17)	0.0006 (13)	0.0016 (16)
C12C	0.0234 (17)	0.020 (2)	0.0176 (16)	−0.0011 (15)	0.0026 (13)	−0.0039 (15)
C13C	0.0261 (17)	0.021 (2)	0.0211 (18)	−0.0011 (16)	0.0033 (14)	−0.0021 (16)
C14C	0.0244 (17)	0.021 (2)	0.0272 (18)	−0.0090 (16)	0.0000 (14)	−0.0031 (16)
C15C	0.0204 (16)	0.028 (2)	0.0204 (17)	−0.0053 (16)	0.0023 (13)	−0.0022 (16)
C1D	0.0336 (18)	0.021 (2)	0.0245 (16)	−0.0005 (18)	0.0056 (14)	0.0027 (17)
C2D	0.0251 (18)	0.033 (3)	0.0262 (17)	−0.0069 (17)	0.0016 (13)	0.0008 (18)

C3D	0.0275 (18)	0.033 (3)	0.0269 (19)	0.0059 (18)	0.0045 (15)	0.0074 (18)
C4D	0.0355 (19)	0.027 (2)	0.0225 (18)	0.0023 (18)	0.0085 (15)	0.0016 (16)
N5D	0.0380 (16)	0.0211 (18)	0.0278 (14)	−0.0065 (16)	−0.0008 (12)	0.0042 (15)
C6D	0.0329 (19)	0.037 (3)	0.034 (2)	−0.0039 (19)	0.0086 (15)	−0.0069 (19)
C7D	0.040 (2)	0.047 (3)	0.0291 (19)	−0.008 (2)	0.0037 (16)	−0.011 (2)
C8D	0.033 (2)	0.056 (3)	0.026 (2)	−0.009 (2)	−0.0012 (16)	−0.002 (2)
C9D	0.0298 (19)	0.039 (3)	0.034 (2)	−0.003 (2)	0.0041 (15)	0.003 (2)
C10D	0.0246 (17)	0.026 (2)	0.0295 (18)	0.0019 (17)	0.0082 (14)	0.0060 (17)
O10D	0.0231 (12)	0.043 (2)	0.0441 (14)	−0.0020 (14)	0.0013 (10)	0.0007 (15)
C16D	0.0240 (18)	0.053 (3)	0.046 (2)	0.015 (2)	0.0161 (17)	0.017 (2)
C11D	0.0279 (17)	0.029 (2)	0.0226 (17)	−0.0019 (17)	0.0088 (13)	0.0008 (17)
C12D	0.0246 (17)	0.022 (2)	0.0218 (17)	−0.0016 (16)	0.0024 (13)	0.0054 (16)
C13D	0.0298 (18)	0.019 (2)	0.0219 (18)	−0.0021 (16)	0.0037 (14)	0.0033 (16)
C14D	0.0274 (17)	0.027 (2)	0.0254 (18)	−0.0060 (17)	0.0081 (14)	0.0018 (17)
C15D	0.0268 (17)	0.028 (2)	0.0266 (18)	−0.0037 (17)	0.0087 (14)	0.0037 (17)
C1E	0.0275 (17)	0.025 (2)	0.0192 (15)	0.0011 (17)	0.0016 (13)	0.0019 (17)
C2E	0.0202 (16)	0.034 (3)	0.0269 (17)	0.0026 (17)	0.0010 (13)	−0.0014 (18)
C3E	0.0225 (17)	0.028 (3)	0.031 (2)	−0.0042 (17)	0.0083 (15)	−0.0063 (17)
C4E	0.0335 (19)	0.023 (2)	0.0279 (19)	−0.0092 (18)	0.0083 (15)	−0.0041 (17)
N5E	0.0329 (15)	0.0176 (17)	0.0314 (15)	0.0048 (15)	0.0010 (12)	−0.0002 (14)
C6E	0.040 (2)	0.031 (3)	0.036 (2)	0.0070 (19)	0.0112 (16)	0.0122 (19)
C7E	0.036 (2)	0.047 (3)	0.0308 (19)	0.013 (2)	0.0108 (16)	0.019 (2)
C8E	0.0306 (19)	0.056 (3)	0.0221 (19)	0.012 (2)	0.0046 (15)	0.003 (2)
C9E	0.0205 (16)	0.040 (3)	0.030 (2)	0.0045 (18)	0.0045 (14)	−0.0006 (18)
C10E	0.0203 (16)	0.023 (2)	0.0262 (17)	0.0049 (16)	0.0052 (13)	−0.0024 (16)
O10E	0.0201 (12)	0.0350 (18)	0.0353 (13)	−0.0030 (13)	−0.0007 (9)	0.0066 (13)
C16E	0.0224 (17)	0.034 (3)	0.044 (2)	−0.0013 (17)	0.0080 (16)	0.008 (2)
C11E	0.0236 (16)	0.025 (2)	0.0219 (16)	−0.0010 (16)	0.0063 (13)	0.0012 (16)
C12E	0.0205 (16)	0.024 (2)	0.0192 (17)	0.0008 (15)	0.0018 (13)	−0.0014 (16)
C13E	0.0253 (18)	0.026 (2)	0.0229 (18)	0.0001 (17)	0.0054 (14)	−0.0035 (17)
C14E	0.0266 (17)	0.027 (2)	0.0237 (18)	0.0058 (16)	0.0048 (14)	−0.0019 (16)
C15E	0.0218 (16)	0.025 (2)	0.0246 (18)	0.0044 (16)	0.0055 (13)	0.0030 (16)
C1F	0.0313 (18)	0.024 (2)	0.0232 (16)	0.0020 (18)	0.0025 (13)	−0.0001 (17)
C2F	0.0265 (17)	0.036 (3)	0.0245 (18)	0.0052 (18)	0.0015 (13)	0.0052 (18)
C3F	0.0266 (18)	0.043 (3)	0.0248 (19)	−0.0035 (18)	0.0060 (15)	0.0058 (19)
C4F	0.038 (2)	0.028 (2)	0.0201 (17)	0.0001 (18)	0.0029 (15)	0.0035 (16)
N5F	0.0378 (16)	0.0209 (18)	0.0315 (15)	0.0066 (16)	0.0119 (12)	0.0106 (15)
C6F	0.0296 (18)	0.036 (3)	0.034 (2)	0.0053 (18)	0.0006 (15)	−0.0094 (19)
C7F	0.036 (2)	0.042 (3)	0.034 (2)	0.010 (2)	0.0062 (16)	−0.006 (2)
C8F	0.034 (2)	0.057 (3)	0.031 (2)	0.012 (2)	0.0127 (17)	0.004 (2)
C9F	0.0280 (18)	0.031 (3)	0.033 (2)	0.0000 (18)	0.0032 (15)	−0.0007 (19)
C10F	0.0243 (17)	0.029 (2)	0.0287 (18)	−0.0003 (17)	−0.0019 (14)	0.0022 (17)
O10F	0.0233 (12)	0.043 (2)	0.0438 (14)	0.0017 (14)	0.0071 (10)	0.0010 (15)
C16F	0.0222 (18)	0.052 (3)	0.036 (2)	−0.0168 (19)	−0.0105 (15)	0.012 (2)
C11F	0.0302 (18)	0.020 (2)	0.0223 (16)	−0.0007 (17)	−0.0021 (13)	−0.0009 (16)
C12F	0.0282 (18)	0.025 (2)	0.0187 (17)	0.0001 (17)	0.0048 (13)	0.0033 (16)
C13F	0.0245 (17)	0.023 (2)	0.0212 (17)	0.0038 (16)	0.0043 (14)	0.0067 (16)
C14F	0.0259 (17)	0.023 (2)	0.0273 (18)	0.0062 (16)	0.0012 (14)	0.0024 (17)

C15F	0.0241 (16)	0.028 (2)	0.0247 (18)	0.0059 (17)	0.0030 (14)	0.0024 (17)

Geometric parameters (Å, º)

C1A—C2A	1.385 (4)	C1D—C2D	1.382 (4)
C1A—C12A	1.391 (4)	C1D—C12D	1.395 (4)
C1A—H1A	0.95	C1D—H1D	0.95
C2A—C3A	1.377 (5)	C2D—C3D	1.382 (5)
C2A—H2A	0.95	C2D—H2D	0.95
C3A—C4A	1.380 (5)	C3D—C4D	1.394 (5)
C3A—H3A	0.95	C3D—H3D	0.95
C4A—C13A	1.391 (4)	C4D—C13D	1.388 (5)
C4A—H4A	0.95	C4D—H4D	0.95
N5A—C13A	1.421 (4)	N5D—C13D	1.417 (4)
N5A—C14A	1.426 (4)	N5D—C14D	1.417 (4)
N5A—H5A	0.88	N5D—H5D	0.88
C6A—C7A	1.388 (5)	C6D—C7D	1.377 (5)
C6A—C14A	1.395 (5)	C6D—C14D	1.386 (5)
C6A—H6A	0.95	C6D—H6D	0.95
C7A—C8A	1.381 (6)	C7D—C8D	1.389 (6)
C7A—H7A	0.95	C7D—H7D	0.95
C8A—C9A	1.375 (5)	C8D—C9D	1.380 (5)
C8A—H8A	0.95	C8D—H8D	0.95
C9A—C15A	1.405 (4)	C9D—C15D	1.396 (4)
C9A—H9A	0.95	C9D—H9D	0.95
C10A—C11A	1.331 (4)	C10D—C11D	1.339 (4)
C10A—O10A	1.405 (4)	C10D—O10D	1.389 (4)
C10A—C15A	1.484 (5)	C10D—C15D	1.485 (5)
O10A—C16A	1.283 (5)	O10D—C16D	1.303 (5)
C16A—H16A	0.98	C16D—H16D	0.98
C16A—H17A	0.98	C16D—H17D	0.98
C16A—H18A	0.98	C16D—H18D	0.98
C11A—C12A	1.479 (4)	C11D—C12D	1.475 (4)
C11A—H11A	0.95	C11D—H11D	0.95
C12A—C13A	1.399 (5)	C12D—C13D	1.402 (5)
C14A—C15A	1.390 (5)	C14D—C15D	1.406 (5)
C1B—C2B	1.378 (4)	C1E—C2E	1.386 (4)
C1B—C12B	1.396 (4)	C1E—C12E	1.388 (4)
C1B—H1B	0.95	C1E—H1E	0.95
C2B—C3B	1.383 (5)	C2E—C3E	1.370 (5)
C2B—H2B	0.95	C2E—H2E	0.95
C3B—C4B	1.395 (5)	C3E—C4E	1.383 (5)
C3B—H3B	0.95	C3E—H3E	0.95
C4B—C13B	1.391 (4)	C4E—C13E	1.390 (4)
C4B—H4B	0.95	C4E—H4E	0.95
N5B—C13B	1.413 (4)	N5E—C14E	1.417 (4)
N5B—C14B	1.415 (4)	N5E—C13E	1.416 (4)
N5B—H5B	0.88	N5E—H5E	0.88

C6B—C14B	1.390 (5)	C6E—C7E	1.383 (5)
C6B—C7B	1.396 (5)	C6E—C14E	1.391 (5)
C6B—H6B	0.95	C6E—H6E	0.95
C7B—C8B	1.372 (5)	C7E—C8E	1.373 (6)
C7B—H7B	0.95	C7E—H7E	0.95
C8B—C9B	1.393 (5)	C8E—C9E	1.386 (5)
C8B—H8B	0.95	C8E—H8E	0.95
C9B—C15B	1.413 (4)	C9E—C15E	1.408 (4)
C9B—H9B	0.95	C9E—H9E	0.95
C10B—C11B	1.338 (4)	C10E—C11E	1.332 (4)
C10B—O10B	1.374 (4)	C10E—O10E	1.373 (4)
C10B—C15B	1.473 (5)	C10E—C15E	1.484 (5)
O10B—C16B	1.414 (4)	O10E—C16E	1.404 (4)
C16B—H16B	0.98	C16E—H16E	0.98
C16B—H17B	0.98	C16E—H17E	0.98
C16B—H18B	0.98	C16E—H18E	0.98
C11B—C12B	1.476 (4)	C11E—C12E	1.479 (4)
C11B—H11B	0.95	C11E—H11E	0.95
C12B—C13B	1.403 (5)	C12E—C13E	1.401 (5)
C14B—C15B	1.396 (5)	C14E—C15E	1.395 (5)
C1C—C2C	1.372 (4)	C1F—C2F	1.389 (4)
C1C—C12C	1.395 (4)	C1F—C12F	1.397 (5)
C1C—H1C	0.95	C1F—H1F	0.95
C2C—C3C	1.393 (5)	C2F—C3F	1.386 (5)
C2C—H2C	0.95	C2F—H2F	0.95
C3C—C4C	1.377 (5)	C3F—C4F	1.391 (5)
C3C—H3C	0.95	C3F—H3F	0.95
C4C—C13C	1.389 (4)	C4F—C13F	1.390 (5)
C4C—H4C	0.95	C4F—H4F	0.95
N5C—C14C	1.422 (4)	N5F—C14F	1.415 (4)
N5C—C13C	1.422 (4)	N5F—C13F	1.423 (4)
N5C—H5C	0.88	N5F—H5F	0.88
C6C—C7C	1.392 (5)	C6F—C7F	1.387 (5)
C6C—C14C	1.389 (5)	C6F—C14F	1.394 (5)
C6C—H6C	0.95	C6F—H6F	0.95
C7C—C8C	1.372 (6)	C7F—C8F	1.380 (6)
C7C—H7C	0.95	C7F—H7F	0.95
C8C—C9C	1.394 (5)	C8F—C9F	1.384 (5)
C8C—H8C	0.95	C8F—H8F	0.95
C9C—C15C	1.411 (4)	C9F—C15F	1.408 (4)
C9C—H9C	0.95	C9F—H9F	0.95
C10C—C11C	1.343 (4)	C10F—C11F	1.341 (4)
C10C—O10C	1.381 (4)	C10F—O10F	1.389 (4)
C10C—C15C	1.471 (5)	C10F—C15F	1.476 (5)
O10C—C16C	1.404 (4)	O10F—C16F	1.311 (5)
C16C—H16C	0.98	C16F—H16F	0.98
C16C—H17C	0.98	C16F—H17F	0.98
C16C—H18C	0.98	C16F—H18F	0.98

C11C—C12C	1.475 (4)	C11F—C12F	1.471 (4)
C11C—H11C	0.95	C11F—H11F	0.95
C12C—C13C	1.406 (5)	C12F—C13F	1.394 (5)
C14C—C15C	1.392 (5)	C14F—C15F	1.395 (5)
C2A—C1A—C12A	122.1 (4)	C2D—C1D—C12D	122.2 (3)
C2A—C1A—H1A	119.0	C2D—C1D—H1D	118.9
C12A—C1A—H1A	119.0	C12D—C1D—H1D	118.9
C3A—C2A—C1A	119.4 (3)	C1D—C2D—C3D	119.4 (3)
C3A—C2A—H2A	120.3	C1D—C2D—H2D	120.3
C1A—C2A—H2A	120.3	C3D—C2D—H2D	120.3
C4A—C3A—C2A	119.9 (3)	C2D—C3D—C4D	119.7 (3)
C4A—C3A—H3A	120.1	C2D—C3D—H3D	120.1
C2A—C3A—H3A	120.1	C4D—C3D—H3D	120.1
C3A—C4A—C13A	120.8 (4)	C3D—C4D—C13D	120.6 (4)
C3A—C4A—H4A	119.6	C3D—C4D—H4D	119.7
C13A—C4A—H4A	119.6	C13D—C4D—H4D	119.7
C13A—N5A—C14A	119.2 (3)	C13D—N5D—C14D	119.5 (3)
C13A—N5A—H5A	120.4	C13D—N5D—H5D	120.3
C14A—N5A—H5A	120.4	C14D—N5D—H5D	120.3
C7A—C6A—C14A	119.9 (4)	C7D—C6D—C14D	121.2 (4)
C7A—C6A—H6A	120.0	C7D—C6D—H6D	119.4
C14A—C6A—H6A	120.0	C14D—C6D—H6D	119.4
C8A—C7A—C6A	120.0 (4)	C6D—C7D—C8D	119.4 (4)
C8A—C7A—H7A	120.0	C6D—C7D—H7D	120.3
C6A—C7A—H7A	120.0	C8D—C7D—H7D	120.3
C9A—C8A—C7A	120.0 (4)	C9D—C8D—C7D	119.9 (3)
C9A—C8A—H8A	120.0	C9D—C8D—H8D	120.0
C7A—C8A—H8A	120.0	C7D—C8D—H8D	120.0
C8A—C9A—C15A	121.2 (4)	C8D—C9D—C15D	121.4 (4)
C8A—C9A—H9A	119.4	C8D—C9D—H9D	119.3
C15A—C9A—H9A	119.4	C15D—C9D—H9D	119.3
C11A—C10A—O10A	122.3 (3)	C11D—C10D—O10D	122.8 (3)
C11A—C10A—C15A	127.0 (3)	C11D—C10D—C15D	127.1 (3)
O10A—C10A—C15A	110.7 (3)	O10D—C10D—C15D	110.1 (3)
C16A—O10A—C10A	119.9 (3)	C16D—O10D—C10D	119.8 (3)
O10A—C16A—H16A	109.5	O10D—C16D—H16D	109.5
O10A—C16A—H17A	109.5	O10D—C16D—H17D	109.5
H16A—C16A—H17A	109.5	H16D—C16D—H17D	109.5
O10A—C16A—H18A	109.5	O10D—C16D—H18D	109.5
H16A—C16A—H18A	109.5	H16D—C16D—H18D	109.5
H17A—C16A—H18A	109.5	H17D—C16D—H18D	109.5
C10A—C11A—C12A	127.2 (3)	C10D—C11D—C12D	126.6 (3)
C10A—C11A—H11A	116.4	C10D—C11D—H11D	116.7
C12A—C11A—H11A	116.4	C12D—C11D—H11D	116.7
C1A—C12A—C13A	117.7 (3)	C1D—C12D—C13D	117.8 (3)
C1A—C12A—C11A	118.5 (3)	C1D—C12D—C11D	118.2 (3)
C13A—C12A—C11A	123.8 (3)	C13D—C12D—C11D	124.0 (3)

C4A—C13A—C12A	120.2 (3)	C4D—C13D—C12D	120.3 (3)
C4A—C13A—N5A	119.0 (3)	C4D—C13D—N5D	118.8 (3)
C12A—C13A—N5A	120.7 (3)	C12D—C13D—N5D	120.8 (3)
C15A—C14A—C6A	120.6 (3)	C6D—C14D—C15D	119.9 (3)
C15A—C14A—N5A	121.7 (3)	C6D—C14D—N5D	118.4 (3)
C6A—C14A—N5A	117.6 (3)	C15D—C14D—N5D	121.6 (3)
C14A—C15A—C9A	118.2 (3)	C9D—C15D—C14D	118.1 (3)
C14A—C15A—C10A	123.3 (3)	C9D—C15D—C10D	119.0 (3)
C9A—C15A—C10A	118.5 (3)	C14D—C15D—C10D	123.0 (3)
C2B—C1B—C12B	122.0 (4)	C2E—C1E—C12E	121.8 (3)
C2B—C1B—H1B	119.0	C2E—C1E—H1E	119.1
C12B—C1B—H1B	119.0	C12E—C1E—H1E	119.1
C1B—C2B—C3B	119.5 (3)	C3E—C2E—C1E	119.6 (3)
C1B—C2B—H2B	120.3	C3E—C2E—H2E	120.2
C3B—C2B—H2B	120.3	C1E—C2E—H2E	120.2
C2B—C3B—C4B	119.9 (3)	C2E—C3E—C4E	119.8 (3)
C2B—C3B—H3B	120.1	C2E—C3E—H3E	120.1
C4B—C3B—H3B	120.1	C4E—C3E—H3E	120.1
C13B—C4B—C3B	120.6 (4)	C3E—C4E—C13E	121.1 (4)
C13B—C4B—H4B	119.7	C3E—C4E—H4E	119.5
C3B—C4B—H4B	119.7	C13E—C4E—H4E	119.5
C13B—N5B—C14B	119.9 (3)	C14E—N5E—C13E	120.0 (3)
C13B—N5B—H5B	120.0	C14E—N5E—H5E	120.0
C14B—N5B—H5B	120.0	C13E—N5E—H5E	120.0
C14B—C6B—C7B	120.6 (4)	C7E—C6E—C14E	120.2 (4)
C14B—C6B—H6B	119.7	C7E—C6E—H6E	119.9
C7B—C6B—H6B	119.7	C14E—C6E—H6E	119.9
C8B—C7B—C6B	119.9 (3)	C8E—C7E—C6E	120.4 (4)
C8B—C7B—H7B	120.0	C8E—C7E—H7E	119.8
C6B—C7B—H7B	120.0	C6E—C7E—H7E	119.8
C7B—C8B—C9B	120.1 (3)	C7E—C8E—C9E	119.8 (3)
C7B—C8B—H8B	120.0	C7E—C8E—H8E	120.1
C9B—C8B—H8B	120.0	C9E—C8E—H8E	120.1
C8B—C9B—C15B	120.8 (4)	C8E—C9E—C15E	121.0 (4)
C8B—C9B—H9B	119.6	C8E—C9E—H9E	119.5
C15B—C9B—H9B	119.6	C15E—C9E—H9E	119.5
C11B—C10B—O10B	122.8 (3)	C11E—C10E—O10E	123.1 (3)
C11B—C10B—C15B	127.9 (3)	C11E—C10E—C15E	127.3 (3)
O10B—C10B—C15B	109.3 (3)	O10E—C10E—C15E	109.6 (3)
C10B—O10B—C16B	118.1 (3)	C10E—O10E—C16E	117.8 (3)
O10B—C16B—H16B	109.5	O10E—C16E—H16E	109.5
O10B—C16B—H17B	109.5	O10E—C16E—H17E	109.5
H16B—C16B—H17B	109.5	H16E—C16E—H17E	109.5
O10B—C16B—H18B	109.5	O10E—C16E—H18E	109.5
H16B—C16B—H18B	109.5	H16E—C16E—H18E	109.5
H17B—C16B—H18B	109.5	H17E—C16E—H18E	109.5
C10B—C11B—C12B	126.0 (3)	C10E—C11E—C12E	126.3 (3)
C10B—C11B—H11B	117.0	C10E—C11E—H11E	116.8

C12B—C11B—H11B	117.0	C12E—C11E—H11E	116.8
C1B—C12B—C13B	118.4 (3)	C1E—C12E—C13E	118.1 (3)
C1B—C12B—C11B	118.2 (3)	C1E—C12E—C11E	118.2 (3)
C13B—C12B—C11B	123.4 (3)	C13E—C12E—C11E	123.6 (3)
C4B—C13B—C12B	119.7 (3)	C4E—C13E—C12E	119.6 (3)
C4B—C13B—N5B	119.4 (3)	C4E—C13E—N5E	119.7 (3)
C12B—C13B—N5B	120.8 (3)	C12E—C13E—N5E	120.5 (3)
C6B—C14B—C15B	120.2 (3)	C6E—C14E—C15E	120.5 (3)
C6B—C14B—N5B	117.8 (3)	C6E—C14E—N5E	118.0 (3)
C15B—C14B—N5B	121.8 (3)	C15E—C14E—N5E	121.4 (3)
C14B—C15B—C9B	118.2 (3)	C14E—C15E—C9E	118.0 (3)
C14B—C15B—C10B	122.8 (3)	C14E—C15E—C10E	123.3 (3)
C9B—C15B—C10B	118.9 (3)	C9E—C15E—C10E	118.6 (3)
C2C—C1C—C12C	122.3 (3)	C2F—C1F—C12F	121.5 (4)
C2C—C1C—H1C	118.8	C2F—C1F—H1F	119.2
C12C—C1C—H1C	118.8	C12F—C1F—H1F	119.2
C1C—C2C—C3C	119.1 (3)	C3F—C2F—C1F	119.7 (4)
C1C—C2C—H2C	120.5	C3F—C2F—H2F	120.1
C3C—C2C—H2C	120.5	C1F—C2F—H2F	120.1
C4C—C3C—C2C	120.0 (3)	C2F—C3F—C4F	119.2 (3)
C4C—C3C—H3C	120.0	C2F—C3F—H3F	120.4
C2C—C3C—H3C	120.0	C4F—C3F—H3F	120.4
C3C—C4C—C13C	120.9 (4)	C3F—C4F—C13F	121.1 (4)
C3C—C4C—H4C	119.6	C3F—C4F—H4F	119.4
C13C—C4C—H4C	119.6	C13F—C4F—H4F	119.4
C14C—N5C—C13C	119.1 (3)	C14F—N5F—C13F	119.0 (3)
C14C—N5C—H5C	120.5	C14F—N5F—H5F	120.5
C13C—N5C—H5C	120.5	C13F—N5F—H5F	120.5
C7C—C6C—C14C	119.8 (4)	C7F—C6F—C14F	120.7 (4)
C7C—C6C—H6C	120.1	C7F—C6F—H6F	119.7
C14C—C6C—H6C	120.1	C14F—C6F—H6F	119.7
C8C—C7C—C6C	120.8 (4)	C8F—C7F—C6F	120.0 (4)
C8C—C7C—H7C	119.6	C8F—C7F—H7F	120.0
C6C—C7C—H7C	119.6	C6F—C7F—H7F	120.0
C7C—C8C—C9C	119.5 (3)	C7F—C8F—C9F	119.6 (3)
C7C—C8C—H8C	120.2	C7F—C8F—H8F	120.2
C9C—C8C—H8C	120.2	C9F—C8F—H8F	120.2
C8C—C9C—C15C	120.8 (4)	C8F—C9F—C15F	121.5 (4)
C8C—C9C—H9C	119.6	C8F—C9F—H9F	119.3
C15C—C9C—H9C	119.6	C15F—C9F—H9F	119.3
C11C—C10C—O10C	122.4 (3)	C11F—C10F—O10F	122.8 (3)
C11C—C10C—C15C	127.6 (3)	C11F—C10F—C15F	126.5 (3)
O10C—C10C—C15C	110.0 (3)	O10F—C10F—C15F	110.7 (3)
C10C—O10C—C16C	118.0 (3)	C16F—O10F—C10F	119.4 (3)
O10C—C16C—H16C	109.5	O10F—C16F—H16F	109.5
O10C—C16C—H17C	109.5	O10F—C16F—H17F	109.5
H16C—C16C—H17C	109.5	H16F—C16F—H17F	109.5
O10C—C16C—H18C	109.5	O10F—C16F—H18F	109.5

H16C—C16C—H18C	109.5	H16F—C16F—H18F	109.5
H17C—C16C—H18C	109.5	H17F—C16F—H18F	109.5
C10C—C11C—C12C	125.8 (3)	C10F—C11F—C12F	127.6 (3)
C10C—C11C—H11C	117.1	C10F—C11F—H11F	116.2
C12C—C11C—H11C	117.1	C12F—C11F—H11F	116.2
C1C—C12C—C13C	117.8 (3)	C13F—C12F—C1F	118.4 (3)
C1C—C12C—C11C	118.5 (3)	C13F—C12F—C11F	123.4 (3)
C13C—C12C—C11C	123.6 (3)	C1F—C12F—C11F	118.3 (3)
C4C—C13C—C12C	119.8 (3)	C4F—C13F—C12F	120.0 (3)
C4C—C13C—N5C	119.5 (3)	C4F—C13F—N5F	118.7 (3)
C12C—C13C—N5C	120.5 (3)	C12F—C13F—N5F	121.2 (3)
C6C—C14C—C15C	120.8 (3)	C6F—C14F—C15F	120.1 (3)
C6C—C14C—N5C	117.8 (3)	C6F—C14F—N5F	118.0 (3)
C15C—C14C—N5C	121.4 (3)	C15F—C14F—N5F	121.9 (3)
C14C—C15C—C9C	118.3 (3)	C14F—C15F—C9F	118.1 (3)
C14C—C15C—C10C	123.4 (3)	C14F—C15F—C10F	123.3 (3)
C9C—C15C—C10C	118.4 (3)	C9F—C15F—C10F	118.5 (3)
C12A—C1A—C2A—C3A	0.3 (5)	C12D—C1D—C2D—C3D	1.1 (5)
C1A—C2A—C3A—C4A	0.1 (5)	C1D—C2D—C3D—C4D	0.2 (5)
C2A—C3A—C4A—C13A	−0.3 (5)	C2D—C3D—C4D—C13D	−0.6 (5)
C14A—C6A—C7A—C8A	−1.0 (6)	C14D—C6D—C7D—C8D	−2.1 (6)
C6A—C7A—C8A—C9A	0.5 (6)	C6D—C7D—C8D—C9D	1.0 (6)
C7A—C8A—C9A—C15A	0.7 (6)	C7D—C8D—C9D—C15D	0.9 (6)
C11A—C10A—O10A—C16A	−14.5 (5)	C11D—C10D—O10D—C16D	−13.9 (5)
C15A—C10A—O10A—C16A	163.5 (3)	C15D—C10D—O10D—C16D	164.4 (3)
O10A—C10A—C11A—C12A	176.7 (3)	O10D—C10D—C11D—C12D	176.9 (3)
C15A—C10A—C11A—C12A	−1.0 (6)	C15D—C10D—C11D—C12D	−1.1 (6)
C2A—C1A—C12A—C13A	−0.5 (5)	C2D—C1D—C12D—C13D	−1.8 (5)
C2A—C1A—C12A—C11A	−177.6 (3)	C2D—C1D—C12D—C11D	−178.2 (3)
C10A—C11A—C12A—C1A	−151.8 (4)	C10D—C11D—C12D—C1D	−151.7 (4)
C10A—C11A—C12A—C13A	31.3 (5)	C10D—C11D—C12D—C13D	32.1 (5)
C3A—C4A—C13A—C12A	0.1 (5)	C3D—C4D—C13D—C12D	−0.1 (5)
C3A—C4A—C13A—N5A	174.7 (3)	C3D—C4D—C13D—N5D	175.5 (3)
C1A—C12A—C13A—C4A	0.3 (5)	C1D—C12D—C13D—C4D	1.3 (5)
C11A—C12A—C13A—C4A	177.2 (3)	C11D—C12D—C13D—C4D	177.5 (3)
C1A—C12A—C13A—N5A	−174.2 (3)	C1D—C12D—C13D—N5D	−174.2 (3)
C11A—C12A—C13A—N5A	2.7 (5)	C11D—C12D—C13D—N5D	2.0 (5)
C14A—N5A—C13A—C4A	124.0 (3)	C14D—N5D—C13D—C4D	123.0 (3)
C14A—N5A—C13A—C12A	−61.3 (4)	C14D—N5D—C13D—C12D	−61.4 (4)
C7A—C6A—C14A—C15A	0.1 (5)	C7D—C6D—C14D—C15D	1.2 (5)
C7A—C6A—C14A—N5A	−176.0 (3)	C7D—C6D—C14D—N5D	−176.2 (3)
C13A—N5A—C14A—C15A	61.0 (4)	C13D—N5D—C14D—C6D	−122.3 (4)
C13A—N5A—C14A—C6A	−122.9 (4)	C13D—N5D—C14D—C15D	60.3 (4)
C6A—C14A—C15A—C9A	1.1 (5)	C8D—C9D—C15D—C14D	−1.7 (5)
N5A—C14A—C15A—C9A	177.0 (3)	C8D—C9D—C15D—C10D	177.0 (3)
C6A—C14A—C15A—C10A	−177.9 (3)	C6D—C14D—C15D—C9D	0.7 (5)
N5A—C14A—C15A—C10A	−1.9 (5)	N5D—C14D—C15D—C9D	178.1 (3)

C8A—C9A—C15A—C14A	−1.5 (5)	C6D—C14D—C15D—C10D	−178.0 (3)
C8A—C9A—C15A—C10A	177.5 (3)	N5D—C14D—C15D—C10D	−0.7 (5)
C11A—C10A—C15A—C14A	−30.3 (6)	C11D—C10D—C15D—C9D	150.1 (4)
O10A—C10A—C15A—C14A	151.8 (3)	O10D—C10D—C15D—C9D	−28.1 (4)
C11A—C10A—C15A—C9A	150.8 (4)	C11D—C10D—C15D—C14D	−31.2 (5)
O10A—C10A—C15A—C9A	−27.2 (4)	O10D—C10D—C15D—C14D	150.6 (3)
C12B—C1B—C2B—C3B	−0.5 (5)	C12E—C1E—C2E—C3E	−0.5 (5)
C1B—C2B—C3B—C4B	−1.7 (5)	C1E—C2E—C3E—C4E	0.7 (5)
C2B—C3B—C4B—C13B	1.9 (5)	C2E—C3E—C4E—C13E	−0.2 (5)
C14B—C6B—C7B—C8B	1.2 (5)	C14E—C6E—C7E—C8E	−1.9 (5)
C6B—C7B—C8B—C9B	−1.2 (5)	C6E—C7E—C8E—C9E	1.3 (5)
C7B—C8B—C9B—C15B	−1.0 (5)	C7E—C8E—C9E—C15E	1.0 (5)
C11B—C10B—O10B—C16B	8.0 (5)	C11E—C10E—O10E—C16E	−10.2 (5)
C15B—C10B—O10B—C16B	−170.1 (3)	C15E—C10E—O10E—C16E	168.6 (3)
O10B—C10B—C11B—C12B	−174.2 (3)	O10E—C10E—C11E—C12E	174.6 (3)
C15B—C10B—C11B—C12B	3.6 (6)	C15E—C10E—C11E—C12E	−3.9 (6)
C2B—C1B—C12B—C13B	2.4 (5)	C2E—C1E—C12E—C13E	−0.3 (5)
C2B—C1B—C12B—C11B	179.6 (3)	C2E—C1E—C12E—C11E	−178.2 (3)
C10B—C11B—C12B—C1B	149.9 (3)	C10E—C11E—C12E—C1E	−148.9 (4)
C10B—C11B—C12B—C13B	−33.1 (5)	C10E—C11E—C12E—C13E	33.2 (5)
C3B—C4B—C13B—C12B	0.0 (5)	C3E—C4E—C13E—C12E	−0.5 (5)
C3B—C4B—C13B—N5B	−176.0 (3)	C3E—C4E—C13E—N5E	174.9 (3)
C1B—C12B—C13B—C4B	−2.1 (5)	C1E—C12E—C13E—C4E	0.7 (5)
C11B—C12B—C13B—C4B	−179.1 (3)	C11E—C12E—C13E—C4E	178.6 (3)
C1B—C12B—C13B—N5B	173.8 (3)	C1E—C12E—C13E—N5E	−174.7 (3)
C11B—C12B—C13B—N5B	−3.2 (5)	C11E—C12E—C13E—N5E	3.2 (5)
C14B—N5B—C13B—C4B	−121.9 (3)	C14E—N5E—C13E—C4E	122.2 (3)
C14B—N5B—C13B—C12B	62.1 (4)	C14E—N5E—C13E—C12E	−62.3 (4)
C7B—C6B—C14B—C15B	1.1 (5)	C7E—C6E—C14E—C15E	0.0 (5)
C7B—C6B—C14B—N5B	177.7 (3)	C7E—C6E—C14E—N5E	−177.2 (3)
C13B—N5B—C14B—C6B	125.3 (3)	C13E—N5E—C14E—C6E	−124.3 (3)
C13B—N5B—C14B—C15B	−58.1 (4)	C13E—N5E—C14E—C15E	58.6 (4)
C6B—C14B—C15B—C9B	−3.2 (5)	C6E—C14E—C15E—C9E	2.3 (5)
N5B—C14B—C15B—C9B	−179.7 (3)	N5E—C14E—C15E—C9E	179.3 (3)
C6B—C14B—C15B—C10B	174.4 (3)	C6E—C14E—C15E—C10E	−175.3 (3)
N5B—C14B—C15B—C10B	−2.1 (5)	N5E—C14E—C15E—C10E	1.7 (5)
C8B—C9B—C15B—C14B	3.2 (5)	C8E—C9E—C15E—C14E	−2.8 (5)
C8B—C9B—C15B—C10B	−174.4 (3)	C8E—C9E—C15E—C10E	174.9 (3)
C11B—C10B—C15B—C14B	31.2 (5)	C11E—C10E—C15E—C14E	−30.7 (5)
O10B—C10B—C15B—C14B	−150.8 (3)	O10E—C10E—C15E—C14E	150.6 (3)
C11B—C10B—C15B—C9B	−151.3 (4)	C11E—C10E—C15E—C9E	151.7 (4)
O10B—C10B—C15B—C9B	26.7 (4)	O10E—C10E—C15E—C9E	−27.0 (4)
C12C—C1C—C2C—C3C	−0.6 (5)	C12F—C1F—C2F—C3F	−0.4 (5)
C1C—C2C—C3C—C4C	−0.2 (5)	C1F—C2F—C3F—C4F	−0.3 (5)
C2C—C3C—C4C—C13C	0.1 (5)	C2F—C3F—C4F—C13F	0.8 (5)
C14C—C6C—C7C—C8C	1.0 (5)	C14F—C6F—C7F—C8F	1.4 (5)
C6C—C7C—C8C—C9C	−0.7 (5)	C6F—C7F—C8F—C9F	−1.0 (5)
C7C—C8C—C9C—C15C	−1.3 (5)	C7F—C8F—C9F—C15F	−0.2 (5)

C11C—C10C—O10C—C16C	10.4 (5)	C11F—C10F—O10F—C16F	13.9 (5)
C15C—C10C—O10C—C16C	−167.4 (3)	C15F—C10F—O10F—C16F	−164.4 (3)
O10C—C10C—C11C—C12C	−174.8 (3)	O10F—C10F—C11F—C12F	−177.0 (3)
C15C—C10C—C11C—C12C	2.7 (6)	C15F—C10F—C11F—C12F	1.1 (6)
C2C—C1C—C12C—C13C	1.3 (4)	C2F—C1F—C12F—C13F	0.7 (5)
C2C—C1C—C12C—C11C	178.5 (3)	C2F—C1F—C12F—C11F	179.0 (3)
C10C—C11C—C12C—C1C	149.5 (3)	C10F—C11F—C12F—C13F	−31.2 (5)
C10C—C11C—C12C—C13C	−33.5 (5)	C10F—C11F—C12F—C1F	150.6 (4)
C3C—C4C—C13C—C12C	0.7 (5)	C3F—C4F—C13F—C12F	−0.5 (5)
C3C—C4C—C13C—N5C	−175.6 (3)	C3F—C4F—C13F—N5F	−175.9 (3)
C1C—C12C—C13C—C4C	−1.4 (4)	C1F—C12F—C13F—C4F	−0.2 (5)
C11C—C12C—C13C—C4C	−178.4 (3)	C11F—C12F—C13F—C4F	−178.4 (3)
C1C—C12C—C13C—N5C	174.8 (3)	C1F—C12F—C13F—N5F	175.1 (3)
C11C—C12C—C13C—N5C	−2.2 (5)	C11F—C12F—C13F—N5F	−3.1 (5)
C14C—N5C—C13C—C4C	−121.6 (3)	C14F—N5F—C13F—C4F	−123.1 (3)
C14C—N5C—C13C—C12C	62.2 (4)	C14F—N5F—C13F—C12F	61.5 (4)
C7C—C6C—C14C—C15C	0.8 (5)	C7F—C6F—C14F—C15F	−0.5 (5)
C7C—C6C—C14C—N5C	177.6 (3)	C7F—C6F—C14F—N5F	176.4 (3)
C13C—N5C—C14C—C6C	123.2 (3)	C13F—N5F—C14F—C6F	122.9 (4)
C13C—N5C—C14C—C15C	−60.0 (4)	C13F—N5F—C14F—C15F	−60.2 (4)
C6C—C14C—C15C—C9C	−2.8 (5)	C6F—C14F—C15F—C9F	−0.6 (5)
N5C—C14C—C15C—C9C	−179.4 (3)	N5F—C14F—C15F—C9F	−177.4 (3)
C6C—C14C—C15C—C10C	176.1 (3)	C6F—C14F—C15F—C10F	177.9 (3)
N5C—C14C—C15C—C10C	−0.6 (5)	N5F—C14F—C15F—C10F	1.1 (5)
C8C—C9C—C15C—C14C	3.0 (5)	C8F—C9F—C15F—C14F	1.0 (5)
C8C—C9C—C15C—C10C	−175.9 (3)	C8F—C9F—C15F—C10F	−177.6 (3)
C11C—C10C—C15C—C14C	31.6 (5)	C11F—C10F—C15F—C14F	30.9 (6)
O10C—C10C—C15C—C14C	−150.7 (3)	O10F—C10F—C15F—C14F	−150.9 (3)
C11C—C10C—C15C—C9C	−149.5 (4)	C11F—C10F—C15F—C9F	−150.6 (4)
O10C—C10C—C15C—C9C	28.2 (4)	O10F—C10F—C15F—C9F	27.6 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5*A*—H5*A*···C11*A*^{i}	0.88	2.54	3.407 (5)	167
N5*B*—H5*B*···C11*B*^{i}	0.88	2.52	3.388 (5)	167
N5*C*—H5*C*···C11*C*^{i}	0.88	2.54	3.403 (5)	167
N5*D*—H5*D*···C11*D*^{i}	0.88	2.53	3.388 (5)	166
N5*E*—H5*E*···C11*E*^{i}	0.88	2.54	3.405 (5)	167
N5*F*—H5*F*···C11*F*^{i}	0.88	2.53	3.391 (5)	167

Symmetry code: (i) *x*, *y*+1, *z*.