

Structure of the mercury(II) mixed-halide (Br/Cl) complex of 2,2'-(5-*tert*-butyl-1,3-phenylene)-bis(1-pentyl-1*H*-benzo[*d*]imidazole)

Varsha Rani,^a Harkesh B. Singh^a and Ray J. Butcher^{b*}^aDepartment of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India, and ^bDepartment of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA. *Correspondence e-mail: rbutter99@yahoo.com

Received 1 February 2017

Accepted 9 February 2017

Edited by M. Zeller, Purdue University, USA

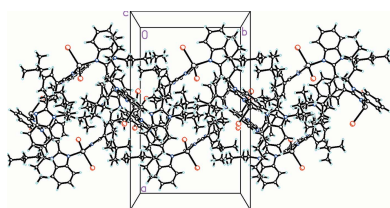
Keywords: crystal structure; single-crystal X-ray study; disorder; mercury coordination polymer; (benzimidazol-2-yl)benzene ligands.**CCDC reference:** 1531940**Supporting information:** this article has supporting information at journals.iucr.org/e

The mercury(II) complex of 2,2'-(5-*tert*-butyl-1,3-phenylene)bis(1-pentyl-1*H*-benzimidazole), namely *catena*-poly[[dihalogenidomercury(II)]- μ -2,2'-(5-*tert*-butyl-1,3-phenylene)bis(1-pentyl-1*H*-benzimidazole)- $\kappa^2 N^3:N^3$], [HgBr_{1.52}Cl_{0.48}(C₃₄H₄₂N₄)], **2**, has a polymeric structure bridging *via* the N atoms from the benzimidazole moieties of the ligand. The compound crystallizes in the orthorhombic space group *Pca*2₁ and is a racemic twin [BASF = 0.402 (9)]. The geometry around the Hg^{II} atom is distorted tetrahedral, with the Hg^{II} atom coordinated to two N atoms, one Br atom, and a fourth coordination site is occupied by a mixed halide (Br/Cl). For the two ligands in the asymmetric unit, there is disorder with one of the two *tert*-butyl groups and benzimidazole moieties showing twofold disorder, with occupancy factors of 0.57 (2):0.43 (2) for the *tert*-butyl group and 0.73 (3):0.27 (3) for the benzimidazole group. In addition, there is threefold disorder for two of the four *n*-pentyl groups, with occupancy factors of 0.669 (4):0.177 (4):0.154 (4) and 0.662 (4):0.224 (4):0.154 (4), respectively. The molecules form a one-dimensional helical polymer propagating in the *b*-axis direction. The helices are held together by intra-strand C—H···Br and C—H···Cl interactions. Each strand is further linked by inter-strand C—H···Br and C—H···Cl interactions. In addition, there are weak C—H···N inter-strand interactions which further stabilize the structural arrangement.

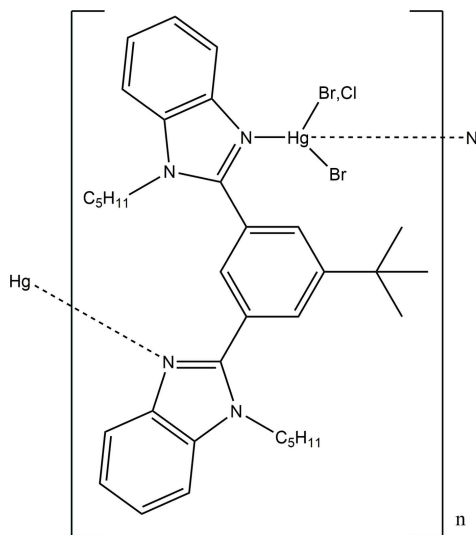
1. Chemical context

During the past few years, metallated complexes of 1,3-bis(1*H*-benzimidazol-2-yl)benzene ligand have been well explored. This ligand is an ideal candidate for metalation due to the presence of two N atoms and one C atom which bind tightly with metal atoms (Carina *et al.*, 1997; Obara *et al.*, 2006; Karlsson *et al.*, 2011; Yang *et al.*, 2012; Tam *et al.*, 2012; Gonzalez, 2014). A highly phosphorescent iridium complex has been reported with the bis(benzimidazol-2-yl)benzene ligand (Obara *et al.*, 2006). Helical and nonhelical copper(I) complexes with bis(benzimidazol-2-yl)benzene have been reported (Rüttimann *et al.*, 1992). A trimeric complex has been obtained through the self assembly of cyclometalated trinuclear palladium(II) complexes (Rüttimann *et al.*, 1993). Dinuclear zinc complexes containing (benzimidazol-2-yl)-benzene based ligands have shown anticancer activities (Xie *et al.*, 2014).

A literature survey of mercury halide complexes with benzimidazole derivatives has shown that they come in two main types: polymeric, bridging either through the halide (Zhang *et al.*, 2015; Li *et al.*, 2007; Shen *et al.*, 2005) or through alternative N atoms from the benzimidazole moieties (Xiao *et*



al., 2009, 2011; Huang *et al.*, 2006; Li *et al.*, 2007, 2012*a,b*; Dey *et al.*, 2013; Du *et al.*, 2011; Chen *et al.*, 2013; Su *et al.*, 2003; Xu *et al.*, 2011), or as discrete molecules (*i.e.* non-polymeric). A structurally related complex has been presented recently (Rani *et al.*, 2017).



In an attempt to synthesize bis[4-*tert*-butyl-2,6-bis(1-pentyl-1*H*-benzimidazol-2-yl)phenyl]mercury (**3**) from [4-*tert*-butyl-2,6-bis(1-pentyl-1*H*-benzimidazol-2-yl)phenyl]mercury(II) chloride ($C_{34}H_{41}N_4HgCl$), **1**, and tetra-*n*-butylammonium bromide ($Bu_4N^+Cl^-$) in dry acetone, the mercury complex of 2,2'-(5-*tert*-butyl-1,3-phenylene)bis(1-pentyl-1*H*-benzimidazole) [$HgBr_{1.52}Cl_{0.48}(C_{34}H_{42}N_4)$], **2**, was isolated unexpectedly (Fig. 1). The procedure for the synthesis of complex **1** will be reported elsewhere.

2. Structural commentary

The title compound crystallizes in the orthorhombic space group $Pca2_1$ and is a racemic twin [$BASF = 0.402(9)$]. The geometry around the Hg^{II} atom is distorted tetrahedral with the Hg^{II} atom coordinated to two N atoms, one Br atom, and a

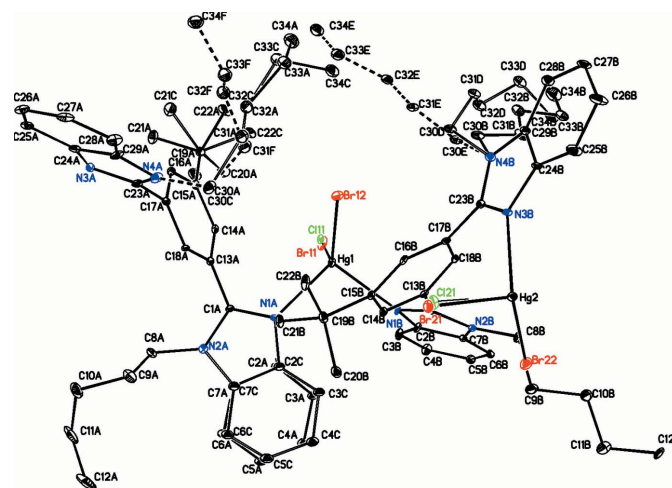


Figure 2
Diagram showing the contents of the asymmetric unit and the disorder in the various moieties. Atomic displacement parameters are shown at the 30% probability level.

fourth coordination site is occupied by a mixed halide (Br/Cl). There are two such sites in the asymmetric unit and in one site, the Br/Cl occupancy is 0.599 (9):0.401 (9) and in the other site the ratio is 0.431 (9):0.569 (9), giving an overall composition (L) $_2HgBr_{1.52}Cl_{0.48}$, where L is 2,2'-(5-*tert*-butyl-1,3-phenylene)bis(1-pentyl-1*H*-benzimidazole). Unlike the case with the recently published structure (Rani *et al.*, 2017) of a related ligand where both coordinating positions are blocked by substituents (Br and *tert*-butyl), even though in the present ligand one position is open for the formation of an Hg—C bond, the basic arrangement is the same as in the previous structure.

For the two ligands in the asymmetric unit, there is considerable disorder, with one of the two *tert*-butyl groups and benzimidazole moieties showing twofold disorder, with occupancy factors of 0.57 (2):0.43 (2) for the *tert*-butyl group and 0.73 (3):0.27 (3) for the benzimidazole group. In addition, there is threefold disorder for two of the four *n*-pentyl groups, with occupancy factors of 0.669 (4):0.177 (4):0.154 (4) and 0.662 (4):0.224 (4):0.154 (4), respectively, as shown in Fig. 2.

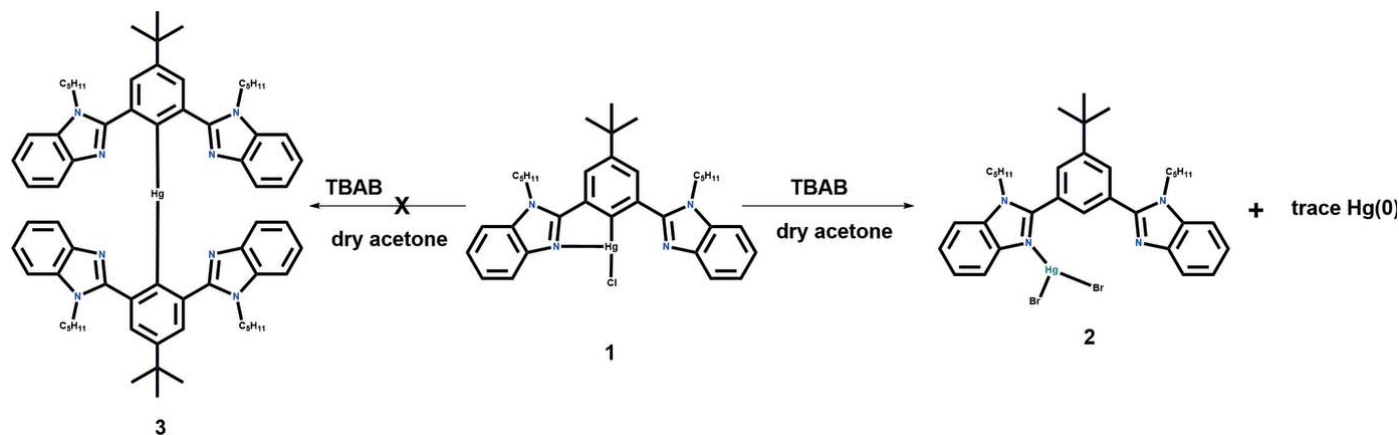


Figure 1
Diagram showing the starting compound, **1**, the title compound, **2**, and the expected product, **3**.

Table 1
Selected geometric parameters (Å, °).

Hg1—N1A	2.313 (7)	Hg2—N3A ⁱ	2.316 (6)
Hg1—N1B	2.343 (6)	Hg2—N3B	2.327 (6)
Hg1—Cl11	2.373 (19)	Hg2—Cl21	2.48 (4)
Hg1—Br12	2.5083 (10)	Hg2—Br22	2.5147 (11)
Hg1—Br11	2.593 (4)	Hg2—Br21	2.57 (2)
N1A—Hg1—N1B	99.4 (3)	N3A ⁱ —Hg2—N3B	97.2 (2)
N1A—Hg1—Cl11	107.1 (6)	N3A ⁱ —Hg2—Cl21	101.7 (8)
N1B—Hg1—Cl11	108.0 (5)	N3B—Hg2—Cl21	105.0 (9)
N1A—Hg1—Br12	115.82 (18)	N3A ⁱ —Hg2—Br22	115.13 (18)
N1B—Hg1—Br12	111.26 (17)	N3B—Hg2—Br22	109.95 (17)
Cl11—Hg1—Br12	114.1 (5)	Cl21—Hg2—Br22	124.1 (7)
N1A—Hg1—Br11	103.9 (2)	N3A ⁱ —Hg2—Br21	105.3 (5)
N1B—Hg1—Br11	105.2 (2)	N3B—Hg2—Br21	107.8 (5)
Br12—Hg1—Br11	119.01 (12)	Br22—Hg2—Br21	119.1 (4)

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

The two sets of Hg—N bond lengths are 2.313 (7)/2.343 (6) and 2.316 (6)/2.327 (6) Å, which span a wider range than that observed (Rani *et al.*, 2017) in a structurally similar complex [2.333 (4)–2.338 (4) Å]. The two sets of Hg—Cl and Hg—Br bond lengths are 2.37 (2)/2.48 (4) (the larger s.u. values are due to the disorder of the anions) and 2.508 (1)/2.593 (4) and 2.515 (1)/2.57 (2) Å, respectively. As mentioned above, the coordination environments are distorted tetrahedral for both Hg^{II} atoms, with bond angles ranging from 97.2 (2) to 124.1 (7)°, values that are more distorted than those found in the analogous complex [100.6 (1)–126.35 (7)°] due to the disorder in the anions.

The discussion of the conformations adopted by the ligand will be restricted to just those of the major components for the disordered moieties where the ligand has adopted a conformation where the two sets of two benzimidazole moieties are not coplanar with each other or their central arene ring. The dihedral angles between the two sets of benzimidazole moieties are 76.4 (3) and 88.0 (2)° (Table 1), while their

dihedral angles with the central ring are 60.1 (3)/59.5 (3) and 50.1 (3)/60.2 (2)°. These values are significantly different from those observed in the related complex (Rani *et al.*, 2017), where the corresponding angles are 54.9 (6) and 65.6 (4)° between the two benzimidazole moieties (two values due to the disorder of one of these moieties) and 55.6 (1) and 89.3 (5)/79.2 (5)° with the central ring. Further, the four pentyl side chains have adopted quite different conformations. This can be seen by examining the dihedral angles of the C atoms in each of these groups. There are four such angles for each, C(from the planar benzimidazole ring)—N—C—C, N—C—C—C, C—C—C—C, and C—C—C—C (last C is a terminal CH₃ group). The four sets of values are –115.6 (11)/–166.7 (11)/76.2 (19)/67.5 (19), 102.2 (12)/–61.5 (15)/–171.9 (13)/173.0 (16)°, 113.4 (10)/162.5 (9)/–174.7 (10)/–179.5 (11) and –104.2 (15)/–172.4 (13)/–78.2 (15)/177.1 (17)°. From these values it can be seen that the first two pentyl groups have adopted a slightly curled-up conformation, while the last two are in a fully extended all-*trans* conformation (Fig. 3).

3. Supramolecular features

The molecules form a one-dimensional helical polymer propagating in the *b* direction (Fig. 4). The helices are held together by intra-strand C—H···Br and C—H···Cl interactions. Each strand is further linked by inter-strand C—H···Br and C—H···Cl interactions. There are inter-strand π – π interactions between the benzimidazole moieties which help stabilize the packing [N1B/N2B/C1B/C2B/C7B···C24A–C29A (symmetry code: $\frac{1}{2} + x, 1 - y, z$) and N3A/N4A/C23A/C24A/C29A···C2B–C7B (symmetry code: $x - \frac{1}{2}, 1 - y, z$)]. In addition, there are weak C—H···N interactions which further stabilize the structural arrangement. Numerical details are given in Table 2.

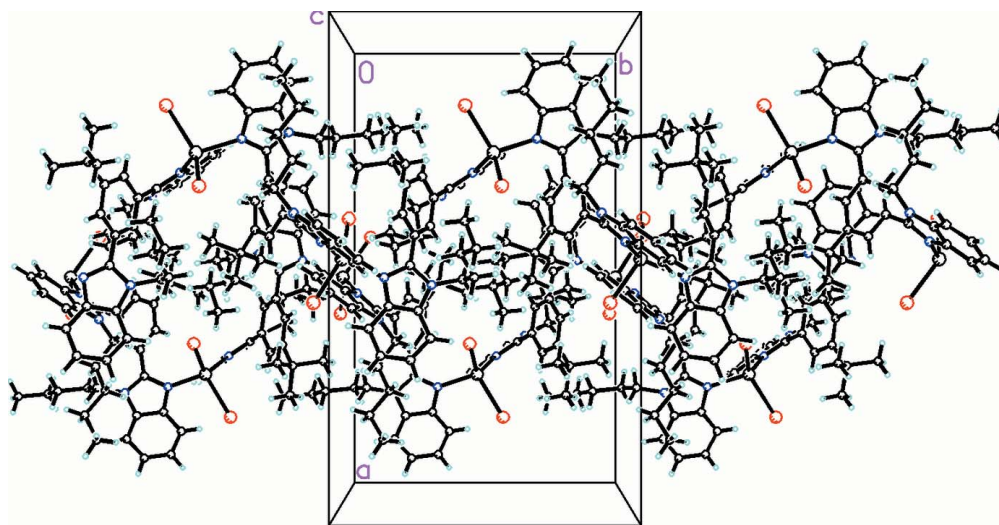


Figure 3

Diagram containing two units of the polymer illustrating its zigzag nature, with H atoms omitted for clarity (symmetry code for generating the second unit: $x, y - 1, z$). Minor components of both the pentyl and benzimidazole disorder, as well as the chloride-anion disorder, have been omitted for clarity. H atoms have also been omitted for clarity. Atomic displacement parameters are shown at the 30% probability level.

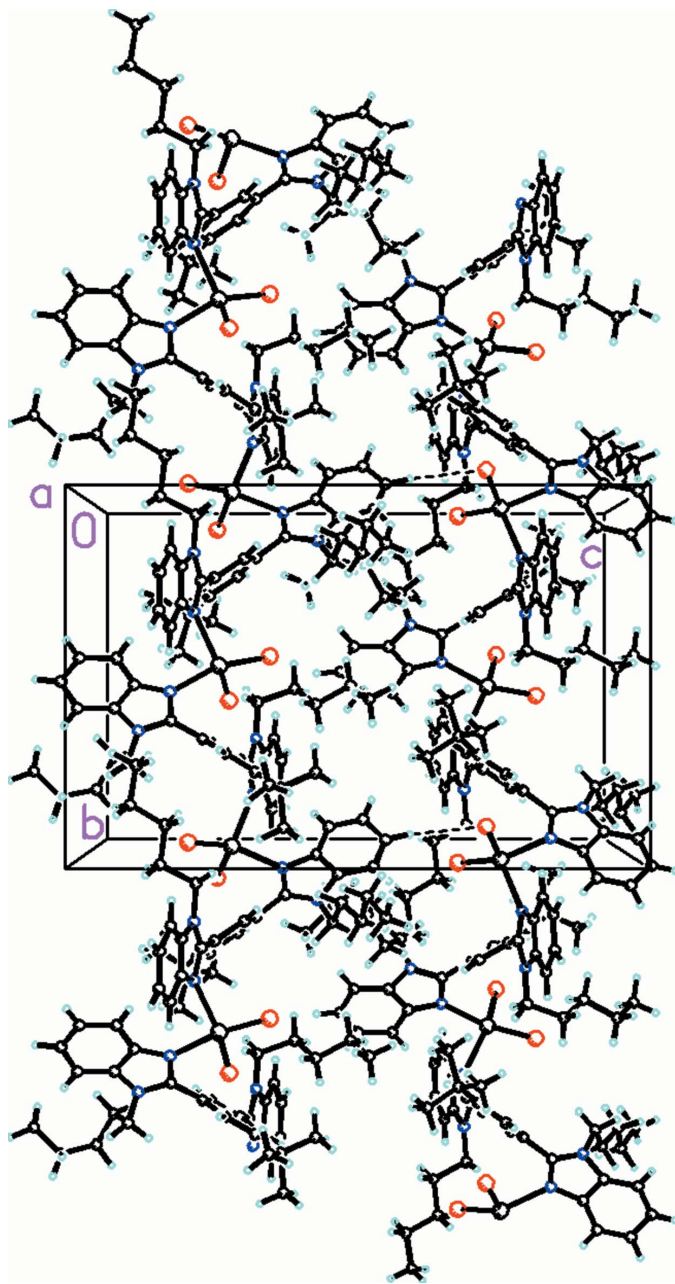


Figure 4
Packing diagram, viewed along the *c* axis, showing two strands of the polymer which propagate in the *b*-axis direction.

4. Database survey

A survey of the structural investigations of mercury halide complexes with benzimidazole derivatives has shown that they come in two main types; polymeric, bridging either through the halide (Zhang *et al.*, 2015; Li *et al.*, 2007; Shen *et al.*, 2005) or through alternative N atoms from the benzimidazole moieties (Xiao *et al.*, 2009, 2011; Huang *et al.*, 2006; Li *et al.*, 2007, 2012*a,b*; Dey *et al.*, 2013; Du *et al.*, 2011; Chen *et al.*, 2013; Su *et al.*, 2003; Xu *et al.*, 2011), or discrete molecules, *i.e.* nonpolymeric (Xiao *et al.*, 2011; Wu *et al.*, 2009; Zhao *et al.*, 2012; Lou *et al.*, 2012; Zhu *et al.*, 2009; Carballo *et al.*, 1993; Yan *et al.*, 2012; Hu *et al.*, 2012, 2015; Ding *et al.*, 2012; Matthews *et al.*, 1998; Manjunatha *et al.*, 2011; Wang *et al.*, 2007, 2009, 2012, 2015; Chen *et al.*, 2014; Su *et al.*, 2003; Quiroz-Castro *et al.*, 2000; Yang & Luo, 2012; He *et al.*, 2012; Bouchouit *et al.*, 2015).

Table 2
Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C3A—H3AA···N1B	0.95	2.45	3.29 (4)	148
C8A—H8AB···Br22 ⁱⁱ	0.99	2.94	3.873 (11)	158
C25A—H25A···Br21 ⁱⁱ	0.95	2.96	3.66 (2)	131
C25A—H25A···Cl21 ⁱⁱⁱ	0.95	2.74	3.45 (3)	132
C28A—H28A···Br11 ⁱⁱⁱ	0.95	2.96	3.793 (12)	147
C28A—H28A···Cl11 ⁱⁱⁱ	0.95	2.86	3.70 (2)	149
C30A—H30B···Br11 ⁱⁱⁱ	0.99	3.04	3.979 (13)	158
C3B—H3BA···Br11	0.95	2.96	3.631 (11)	129
C6B—H6BA···Br21 ^{iv}	0.95	2.88	3.75 (2)	153
C6B—H6BA···Cl21 ^{iv}	0.95	2.89	3.73 (4)	149
C25B—H25B···N3A ⁱ	0.95	2.56	3.332 (14)	139
C30D—H30G···Br12	0.99	3.06	3.95 (5)	150

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

et al., 1998; Manjunatha *et al.*, 2011; Wang *et al.*, 2007, 2009, 2012, 2015; Chen *et al.*, 2014; Su *et al.*, 2003; Quiroz-Castro *et al.*, 2000; Yang & Luo, 2012; He *et al.*, 2012; Bouchouit *et al.*, 2015).

5. Synthesis and crystallization

To a solution of **1** (0.5 g, 0.67 mmol) in dry acetone was added tetra-*n*-butylammonium bromide (0.26 g, 0.82 mmol) at room temperature. The reaction mixture was refluxed for 3 h under an inert atmosphere of N₂ and then filtered through Whatman filter paper. The residue contained shiny mercury particles which could be witnessed with the naked eye and the solvent was evaporated from the filtrate and washed with petroleum ether and then with diethyl ether. The compound was dried under *vacuo*. Colorless plate-shaped single crystals were obtained from DMSO at 291 K (yield 18%, 0.21 g). ¹H NMR (500 MHz, DMSO): δ 7.96–7.93 (*m*, 3H), 7.74 (*d*, *J* = 7.9 Hz, 2H), 7.70 (*d*, *J* = 7.9 Hz, 2H), 7.33–7.26 (*m*, 4H), 4.35 (*t*, *J* = 7.4 Hz, 4H), 1.72 (*m*, 4H), 1.42 (*s*, 9 H), 1.15–0.93 (*m*, 8H), 0.71 (*t*, *J* = 6.8 Hz, 6H). Analysis calculated for C₃₄H₄₂Br_{1.52}Cl_{0.48}HgN₄: C 48.33, H 5.01, N 6.63%; found: C 49.73, H 5.14, N 6.84%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The title compound was refined as a racemic twin [BASF = 0.402 (9)]. The H atoms were positioned geometrically and refined as riding, with C—H = 0.95–0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ otherwise. For the two ligands in the asymmetric unit, there is considerable disorder with one of the two *tert*-butyl groups and benzimidazole moieties showing twofold disorder, with occupancy factors of 0.57 (2):0.43 (2) for the *tert*-butyl group and 0.73 (3):0.27 (3) for the benzimidazole group. The displacement parameters of the disordered *tert*-butyl group were restrained to be similar (SIMU command). One C atom (C22C) from the minor component was additionally restrained to be close to isotropic (ISOR 0.005 command). The two components of the benzimidazole moiety were restrained to be planar using the FLAT command and

Table 3
Experimental details.

Crystal data	
Chemical formula	[HgBr _{1.52} Cl _{0.48} (C ₃₄ H ₄₂ N ₄)]
<i>M_r</i>	845.56
Crystal system, space group	Orthorhombic, <i>Pca</i> 2 ₁
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	22.8887 (14), 13.8830 (8), 21.1396 (12)
<i>V</i> (Å ³)	6717.4 (7)
<i>Z</i>	8
Radiation type	Cu <i>K</i> α
<i>μ</i> (mm ⁻¹)	10.90
Crystal size (mm)	0.19 × 0.17 × 0.07
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Sheldrick, 1996)
<i>T_{min}</i> – <i>T_{max}</i>	0.394, 0.753
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	93252, 11762, 11431
<i>R_{int}</i>	0.043
(sin θ/λ) _{max} (Å ⁻¹)	0.596
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.029, 0.069, 1.14
No. of reflections	11762
No. of parameters	997
No. of restraints	888
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	1.38, -0.85
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.402 (9)

Computer programs: *APEX2* (Bruker, 2005), *SAINT* (Bruker, 2002), *SUPERFLIP* (Palatinus & Chapuis, 2007), *SHELXL2016* (Sheldrick, 2015) and *SHELXTL* (Sheldrick, 2008).

their metrical and displacement parameters were restrained using the SIMU and SADI commands in *SHELXL2016* (Sheldrick, 2015). In addition, there is threefold disorder (occupancies summed to unity using the SUMP command) for two of the four *n*-pentyl groups, with occupancy factors of 0.669 (4):0.177 (4):0.154 (4) and 0.662 (4):0.224 (4):0.154 (4), respectively. For one pentyl group, some atoms (C30A–C32A and C30C–C32C) of two of the three components were refined as overlapping (using EXYZ commands). For the other disordered pentyl group, all atoms of all three components adopt independent conformations. One of the occupancy rates (of the least prevalent moieties *E* and *F*) is shared between the two disordered sites due to mutually exclusive overlap of atoms.

Acknowledgements

RJB is grateful to NSF and the Partnership for Reduced Dimensional Materials for partial funding of this research, the Howard University Nanoscience Facility for access to liquid nitrogen, and the NSF–MRI program for funds to purchase the X-ray diffractometer. HBS is grateful to DST, New Delhi, for a J. C. Bose National Fellowship. VR gratefully acknowledges the Council of Scientific and Industrial Research (CSIR), New Delhi, for a Senior Research Fellowship.

Funding information

Funding for this research was provided by: National Science Foundation, Directorate for Mathematical and Physical Sciences (award No. 1205608); National Science Foundation (award No. CHE0619278).

References

- Bouchouit, M., Benzerka, S., Bouraiou, A., Merazig, H., Belfaitah, A. & Bouacida, S. (2015). *Acta Cryst.* **E71**, m253–m254.
- Bruker (2002). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2005). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Carballo, R., Castineiras, A., Conde, M. C. G. & Hiller, W. (1993). *Polyhedron*, **12**, 1655–1660.
- Carina, R. F., Williams, A. F. & Bernardinelli, G. (1997). *J. Organomet. Chem.* **548**, 45–48.
- Chen, Y., Chen, C., Chen, H., Cao, T., Yue, Z., Liu, X. & Niu, Y. (2013). *Synth. React. Inorg. Met.-Org. Nano-Met. Chem.* **43**, 1307–1310.
- Chen, S., Fan, R.-Q., Wang, X.-M. & Yang, Y.-L. (2014). *CrystEngComm*, **16**, 6114–6125.
- Dey, A., Mandal, S. K. & Biradha, K. (2013). *CrystEngComm*, **15**, 9769–9778.
- Ding, Y., Zhou, X., Jin, G., Zhao, D. & Meng, X. (2012). *Synth. React. Inorg. Met.-Org. Nano-Met. Chem.* **42**, 438–443.
- Du, J.-L., Wei, Z.-Z. & Hu, T.-L. (2011). *Solid State Sci.* **13**, 1256–1260.
- Gonzalez, A. D. (2014). *Organometallics*, **33**, 868–875.
- He, C.-J., Zu, E.-P. & Zhou, X.-J. (2012). *Z. Kristallogr. New Cryst. Struct.* **227**, 445–446.
- Hu, J. Y., Liao, C. L., Hu, L. L., Zhang, C. C., Chen, S. F. & Zhao, J. (2015). *Russ. J. Coord. Chem.* **41**, 212–219.
- Hu, J., Liao, C., Zhao, J. & Haipeng Zhao, H. (2012). *Z. Kristallogr. New Cryst. Struct.* **227**, 69–70.
- Huang, M., Liu, P., Chen, Y., Wang, J. & Liu, Z. (2006). *J. Mol. Struct.* **788**, 211–217.
- Karlsson, E. A., Lee, B., Åkermark, T., Johnston, E. V., Kärkäs, M. D., Sun, J., Hansson, Ö., Bäckvall, J. & Åkermark, B. (2011). *Angew. Chem. Int. Ed.* **50**, 11715–11718.
- Li, J., Li, X., Lu, H., Zhu, Y., Sun, H., Guo, Y., Yue, Z., Zhao, J., Tang, M., Hou, H., Fan, Y. & Chang, J. (2012b). *Inorg. Chim. Acta*, **384**, 163–169.
- Li, Y., Liu, Q.-K., Ma, J.-P. & Dong, Y.-B. (2012a). *Acta Cryst.* **C68**, m152–m155.
- Li, X.-P., Zhang, J.-Y., Liu, Y., Pan, M., Zheng, S.-R., Kang, B.-S. & Cheng-Yong Su, C.-Y. (2007). *Inorg. Chim. Acta*, **360**, 2990–2996.
- Lou, S.-F., Wang, Q. & Ding, J. (2012). *Z. Kristallogr. New Cryst. Struct.* **227**, 105–106.
- Manjunatha, M. N., Dikundwar, A. G. & Nagasundara, K. R. (2011). *Polyhedron*, **30**, 1299–1304.
- Matthews, C. J., Clegg, W., Heath, S. L., Martin, N. C., Hill, M. N. S. & Lockhart, J. C. (1998). *Inorg. Chem.* **37**, 199–207.
- Obara, S., Itabashi, M., Okuda, F., Tamaki, S., Tanabe, Y., Ishii, Y., Nozaki, K. & Haga, M. (2006). *Inorg. Chem.* **45**, 8907–8921.
- Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.
- Quiroz-Castro, E., Bernes, S., Barba-Behrens, N., Tapia-Benavides, R., Contreras, R. & Noth, H. (2000). *Polyhedron*, **19**, 1479–1484.
- Rani, V., Singh, H. B. & Butcher, R. J. (2017). *Acta Cryst.* **E73**, 341–344.
- Rüttimann, S., Bernardinelli, G. & Williams, A. F. (1993). *Angew. Chem. Int. Ed.* **32**, 392–394.
- Rüttimann, S., Pigué, C., Bernardinelli, G., Bocquet, B. & Williams, A. F. (1992). *J. Am. Chem. Soc.* **114**, 4230–4237.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Shen, Y.-H., Liu, J.-G. & Xu, D.-J. (2005). *Acta Cryst.* **E61**, m1880–m1882.
- Su, C.-Y., Goforth, A. M., Smith, M. D. & zur Loye, H.-C. (2003). *Inorg. Chem.* **42**, 5685–5692.
- Tam, A. Y. Y., Tsang, D. P. K., Chan, M. Y., Zhu, N. & Yam, V. W. W. (2012). *Chem. Commun.* **47**, 3383–3385.
- Wang, Q., Fu, Z.-Y. & Yu, L.-M. (2012). *Acta Cryst.* **E68**, m44.
- Wang, X.-F., Lv, Y., Su, Z., Okamura, T., Wu, G., Sun, W.-Y. & Ueyama, N. (2007). *Z. Anorg. Allg. Chem.* **633**, 2695–2700.
- Wang, J.-J., Yan, L.-F., Li, Z.-X., Chang, Z., Hu, T.-L. & Bu, X.-H. (2009). *Inorg. Chim. Acta*, **362**, 3147–3154.
- Wang, X., Yang, H.-Y., Zhang, C., Yuan, J. & Yang, H.-X. (2015). *Z. Kristallogr. New Cryst. Struct.* **230**, 361–362.
- Wu, J., Yang, J. & Pan, F. (2009). *Acta Cryst.* **E65**, m829.
- Xiao, B., Li, W., Hou, H. & Fan, Y. (2009). *J. Coord. Chem.* **62**, 1630–1637.
- Xiao, B., Yang, L.-J., Xiao, H.-Y. & Fang, S.-M. (2011). *J. Coord. Chem.* **64**, 4408–4420.
- Xie, Q., Liu, S., Li, X., Wu, Q., Luo, Z., Fu, X., Cao, W., Lan, G., Li, D., Zheng, W. & Chen, T. (2014). *Dalton Trans.* **43**, 6973–6976.
- Xu, C., Wang, X., Ding, D., Hou, H. & Fan, Y. (2011). *Inorg. Chem. Commun.* **14**, 1410–1413.
- Yan, S., Jin, G., Yang, Y., Su, X. & Meng, X. (2012). *Synth. React. Inorg. Met.-Org. Nano-Met. Chem.* **42**, 678–684.
- Yang, G.-Y. & Luo, L.-X. (2012). *Z. Kristallogr. New Cryst. Struct.* **227**, 441–442.
- Yang, W. W., Zhong, Y. W., Yoshikawa, S., Shao, J. Y., Masaoka, S., Sakai, K., Yao, J. & Haga, M. (2012). *Inorg. Chem.* **51**, 890–899.
- Zhang, Z., Feng, Y.-F., Wei, Q.-Y., Hu, K., Chen, Z.-L. & Liang, F.-P. (2015). *CrystEngComm*, **17**, 6724–6735.
- Zhao, J., Li, S., Chen, S., Bai, Y. & Hu, J. (2012). *J. Coord. Chem.* **65**, 1201–1211.
- Zhu, X.-W., Xiao, B., Yin, Z.-G., Qian, H.-Y. & Li, G.-S. (2009). *Acta Cryst.* **E65**, m912.

supporting information

Acta Cryst. (2017). E73, 423–428 [https://doi.org/10.1107/S2056989017002183]

Structure of the mercury(II) mixed-halide (Br/Cl) complex of 2,2'-(5-*tert*-butyl-1,3-phenylene)bis(1-pentyl-1*H*-benzo[*d*]imidazole)

Varsha Rani, Harkesh B. Singh and Ray J. Butcher

Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2002); program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

catena-Poly[[di(brimido/chlorido)mercury(II)]- μ -2,2'-(5-*tert*-butyl-1,3-phenylene)bis(1-pentyl-1*H*-benzimidazole)- κ^2 N³:N³]

Crystal data

[HgBr_{1.52}Cl_{0.48}(C₃₄H₄₂N₄)]

M_r = 845.56

Orthorhombic, *Pca*2₁

a = 22.8887 (14) Å

b = 13.8830 (8) Å

c = 21.1396 (12) Å

V = 6717.4 (7) Å³

Z = 8

F(000) = 3322

D_x = 1.672 Mg m⁻³

Cu *Kα* radiation, λ = 1.54184 Å

Cell parameters from 9060 reflections

θ = 3.7–66.7°

μ = 10.90 mm⁻¹

T = 100 K

Plate, colourless

0.19 × 0.17 × 0.07 mm

Data collection

Bruker APEXII CCD
diffractometer

ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

T_{min} = 0.394, *T_{max}* = 0.753

93252 measured reflections

11762 independent reflections

11431 reflections with *I* > 2σ(*I*)

R_{int} = 0.043

θ_{max} = 66.8°, θ_{min} = 3.7°

h = -27→26

k = -16→16

l = -25→24

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.029

wR(*F*²) = 0.069

S = 1.14

11762 reflections

997 parameters

888 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0061*P*)² + 31.5501*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.005

Δρ_{max} = 1.38 e Å⁻³

Δρ_{min} = -0.85 e Å⁻³

Absolute structure: Refined as an inversion twin

Absolute structure parameter: 0.402 (9)

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.

Refinement. Refined as a 2-component inversion twin

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Hg1	0.73599 (2)	0.47092 (2)	0.25318 (2)	0.02440 (9)	
Hg2	0.51919 (2)	-0.02075 (2)	0.26809 (2)	0.02425 (9)	
Br12	0.66545 (5)	0.44471 (7)	0.34233 (5)	0.0370 (2)	
Br22	0.60239 (5)	-0.03762 (8)	0.19119 (5)	0.0445 (3)	
Br11	0.83121 (16)	0.5668 (4)	0.2745 (3)	0.0346 (9)	0.599 (9)
Br21	0.4296 (10)	0.0792 (15)	0.2364 (8)	0.0278 (19)	0.431 (9)
Cl11	0.8204 (7)	0.5600 (15)	0.2819 (12)	0.0346 (9)	0.401 (9)
Cl21	0.4287 (19)	0.072 (3)	0.2464 (15)	0.0278 (19)	0.569 (9)
N1A	0.6978 (3)	0.5423 (5)	0.1634 (3)	0.0244 (15)	
N2A	0.6527 (4)	0.6503 (6)	0.1029 (4)	0.0329 (17)	
N3A	0.4820 (3)	0.8355 (5)	0.3065 (3)	0.0212 (14)	
N4A	0.4668 (4)	0.6774 (6)	0.3121 (4)	0.034 (2)	
C1A	0.6660 (4)	0.6220 (6)	0.1630 (4)	0.0216 (17)	
C2A	0.7011 (14)	0.511 (3)	0.1012 (13)	0.032 (4)	0.27 (3)
C3A	0.7268 (19)	0.429 (3)	0.0766 (17)	0.036 (4)	0.27 (3)
H3AA	0.745915	0.382720	0.102702	0.044*	0.27 (3)
C4A	0.723 (2)	0.417 (3)	0.0106 (17)	0.042 (4)	0.27 (3)
H4AA	0.738836	0.361701	-0.009104	0.051*	0.27 (3)
C5A	0.696 (2)	0.486 (3)	-0.0251 (18)	0.043 (4)	0.27 (3)
H5AA	0.695603	0.476618	-0.069650	0.052*	0.27 (3)
C6A	0.6696 (19)	0.567 (3)	-0.002 (2)	0.039 (4)	0.27 (3)
H6AA	0.650217	0.611915	-0.028707	0.047*	0.27 (3)
C7A	0.673 (2)	0.579 (3)	0.064 (2)	0.035 (4)	0.27 (3)
C2C	0.7089 (6)	0.5217 (12)	0.0993 (7)	0.032 (2)	0.73 (3)
C3C	0.7434 (8)	0.4511 (14)	0.0700 (7)	0.036 (3)	0.73 (3)
H3CA	0.764338	0.405323	0.094426	0.043*	0.73 (3)
C4C	0.7461 (10)	0.4498 (13)	0.0038 (7)	0.043 (3)	0.73 (3)
H4CA	0.769263	0.402372	-0.016718	0.052*	0.73 (3)
C5C	0.7163 (9)	0.5152 (14)	-0.0319 (7)	0.044 (3)	0.73 (3)
H5CA	0.717806	0.510586	-0.076686	0.053*	0.73 (3)
C6C	0.6840 (8)	0.5876 (14)	-0.0047 (8)	0.040 (3)	0.73 (3)
H6CA	0.665240	0.635417	-0.029569	0.048*	0.73 (3)
C7C	0.6800 (8)	0.5878 (12)	0.0614 (8)	0.036 (3)	0.73 (3)
C8A	0.6258 (5)	0.7407 (8)	0.0829 (5)	0.043 (3)	
H8AA	0.651868	0.772989	0.052158	0.052*	
H8AB	0.621789	0.783556	0.120103	0.052*	
C9A	0.5670 (5)	0.7270 (11)	0.0533 (6)	0.058 (4)	
H9A1	0.538239	0.709685	0.086429	0.070*	

H9A2	0.568784	0.673280	0.022563	0.070*	
C10A	0.5470 (7)	0.8182 (15)	0.0197 (7)	0.089 (6)	
H10A	0.554632	0.874029	0.047668	0.107*	
H10B	0.504323	0.814408	0.012834	0.107*	
C11A	0.5770 (8)	0.8360 (17)	-0.0441 (8)	0.102 (8)	
H11A	0.566321	0.901378	-0.058928	0.122*	
H11B	0.619796	0.835147	-0.037520	0.122*	
C12A	0.5624 (7)	0.7661 (18)	-0.0949 (7)	0.103 (8)	
H12A	0.519933	0.758753	-0.097678	0.154*	
H12B	0.580235	0.703615	-0.085154	0.154*	
H12C	0.577564	0.789703	-0.135416	0.154*	
C13A	0.6456 (4)	0.6727 (6)	0.2197 (4)	0.0258 (19)	
C14A	0.6867 (4)	0.7111 (5)	0.2622 (4)	0.0249 (17)	
H14A	0.727217	0.701597	0.254546	0.030*	
C15A	0.6689 (4)	0.7630 (6)	0.3156 (4)	0.028 (2)	
C16A	0.6096 (4)	0.7737 (6)	0.3256 (4)	0.0258 (19)	
H16A	0.596773	0.809324	0.361339	0.031*	
C17A	0.5682 (4)	0.7346 (6)	0.2854 (4)	0.0223 (18)	
C18A	0.5862 (4)	0.6849 (6)	0.2315 (4)	0.0220 (17)	
H18A	0.558102	0.659552	0.202911	0.026*	
C19A	0.7129 (5)	0.8058 (8)	0.3625 (5)	0.035 (2)	
C20A	0.7774 (9)	0.794 (2)	0.3430 (11)	0.056 (5)	0.573 (19)
H20A	0.785422	0.834713	0.306063	0.084*	0.573 (19)
H20B	0.785065	0.726650	0.332412	0.084*	0.573 (19)
H20C	0.802608	0.813832	0.378150	0.084*	0.573 (19)
C21A	0.7029 (9)	0.9158 (13)	0.3683 (12)	0.046 (5)	0.573 (19)
H21A	0.732492	0.943457	0.396455	0.069*	0.573 (19)
H21B	0.663934	0.927903	0.385666	0.069*	0.573 (19)
H21C	0.706074	0.945532	0.326377	0.069*	0.573 (19)
C22A	0.7053 (12)	0.763 (2)	0.4258 (10)	0.063 (6)	0.573 (19)
H22A	0.710394	0.693303	0.423325	0.094*	0.573 (19)
H22B	0.666024	0.777947	0.441571	0.094*	0.573 (19)
H22C	0.734459	0.790368	0.454767	0.094*	0.573 (19)
C20C	0.7617 (16)	0.848 (3)	0.3303 (15)	0.057 (6)	0.427 (19)
H20D	0.792848	0.861297	0.360873	0.085*	0.427 (19)
H20E	0.749512	0.907867	0.309942	0.085*	0.427 (19)
H20F	0.776155	0.802804	0.298194	0.085*	0.427 (19)
C21C	0.6807 (14)	0.870 (2)	0.4101 (16)	0.061 (7)	0.427 (19)
H21D	0.650612	0.832825	0.431885	0.092*	0.427 (19)
H21E	0.662311	0.924245	0.387547	0.092*	0.427 (19)
H21F	0.708620	0.895641	0.441063	0.092*	0.427 (19)
C22C	0.7342 (11)	0.717 (2)	0.4038 (12)	0.042 (5)	0.427 (19)
H22D	0.767265	0.737330	0.430250	0.062*	0.427 (19)
H22E	0.746442	0.664732	0.375940	0.062*	0.427 (19)
H22F	0.702144	0.695380	0.430944	0.062*	0.427 (19)
C23A	0.5062 (4)	0.7496 (6)	0.2999 (4)	0.0256 (19)	
C24A	0.4243 (4)	0.8198 (7)	0.3246 (4)	0.027 (2)	
C25A	0.3788 (4)	0.8842 (8)	0.3388 (4)	0.032 (2)	

H25A	0.384475	0.951959	0.337494	0.038*	
C26A	0.3256 (4)	0.8445 (8)	0.3546 (5)	0.036 (2)	
H26A	0.293990	0.885989	0.364851	0.044*	
C27A	0.3170 (5)	0.7458 (9)	0.3560 (5)	0.041 (3)	
H27A	0.279136	0.722255	0.366122	0.049*	
C28A	0.3599 (5)	0.6809 (8)	0.3436 (5)	0.040 (3)	
H28A	0.353422	0.613343	0.345219	0.048*	
C29A	0.4149 (5)	0.7210 (7)	0.3280 (5)	0.035 (2)	
C30A	0.4780 (6)	0.5738 (7)	0.3149 (5)	0.047 (2)	0.669 (4)
H30A	0.515077	0.559681	0.292699	0.057*	0.669 (4)
H30B	0.446264	0.539475	0.292500	0.057*	0.669 (4)
C31A	0.4820 (7)	0.5352 (9)	0.3840 (6)	0.048 (2)	0.669 (4)
H31A	0.444301	0.547779	0.405430	0.057*	0.669 (4)
H31B	0.487401	0.464457	0.382378	0.057*	0.669 (4)
C32A	0.5307 (6)	0.5780 (9)	0.4239 (6)	0.050 (2)	0.669 (4)
H32A	0.522451	0.647020	0.431602	0.060*	0.669 (4)
H32B	0.568025	0.573400	0.400524	0.060*	0.669 (4)
C33A	0.5368 (10)	0.5255 (14)	0.4880 (8)	0.054 (4)	0.669 (4)
H33A	0.501421	0.536933	0.513971	0.065*	0.669 (4)
H33B	0.540386	0.455297	0.480796	0.065*	0.669 (4)
C34A	0.5902 (9)	0.5620 (18)	0.5228 (10)	0.069 (5)	0.669 (4)
H34A	0.586961	0.631841	0.528797	0.103*	0.669 (4)
H34B	0.625269	0.547591	0.497989	0.103*	0.669 (4)
H34C	0.592885	0.530354	0.564120	0.103*	0.669 (4)
C30C	0.4780 (6)	0.5738 (7)	0.3149 (5)	0.047 (2)	0.177 (4)
H30E	0.515077	0.559681	0.292699	0.057*	0.177 (4)
H30F	0.446264	0.539475	0.292500	0.057*	0.177 (4)
C31C	0.4820 (7)	0.5352 (9)	0.3840 (6)	0.048 (2)	0.177 (4)
H31E	0.444301	0.547779	0.405430	0.057*	0.177 (4)
H31F	0.487401	0.464457	0.382378	0.057*	0.177 (4)
C32C	0.5307 (6)	0.5780 (9)	0.4239 (6)	0.050 (2)	0.177 (4)
H32E	0.522609	0.648012	0.425432	0.060*	0.177 (4)
H32F	0.566630	0.570469	0.398389	0.060*	0.177 (4)
C33C	0.548 (4)	0.550 (4)	0.4915 (17)	0.052 (4)	0.177 (4)
H33E	0.580660	0.591743	0.506019	0.062*	0.177 (4)
H33F	0.514593	0.559825	0.520391	0.062*	0.177 (4)
C34C	0.567 (3)	0.447 (4)	0.492 (3)	0.054 (8)	0.177 (4)
H34D	0.599136	0.437561	0.462772	0.080*	0.177 (4)
H34E	0.533746	0.406027	0.479784	0.080*	0.177 (4)
H34F	0.579278	0.429341	0.535156	0.080*	0.177 (4)
C30F	0.4780 (6)	0.5738 (7)	0.3149 (5)	0.047 (2)	0.154 (3)
H30K	0.499902	0.553477	0.276837	0.057*	0.154 (3)
H30L	0.440435	0.538498	0.315708	0.057*	0.154 (3)
C31F	0.513 (2)	0.550 (5)	0.3741 (15)	0.050 (3)	0.154 (3)
H31K	0.513851	0.478893	0.380099	0.060*	0.154 (3)
H31L	0.554043	0.571619	0.368411	0.060*	0.154 (3)
C32F	0.488 (2)	0.597 (5)	0.4327 (19)	0.051 (4)	0.154 (3)
H32K	0.482928	0.666949	0.425206	0.061*	0.154 (3)

H32L	0.514504	0.588202	0.468891	0.061*	0.154 (3)
C33F	0.428 (3)	0.552 (4)	0.448 (3)	0.051 (5)	0.154 (3)
H33K	0.402891	0.553032	0.410377	0.061*	0.154 (3)
H33L	0.433376	0.484577	0.461783	0.061*	0.154 (3)
C34F	0.399 (3)	0.608 (6)	0.501 (3)	0.057 (13)	0.154 (3)
H34P	0.425443	0.611499	0.537044	0.085*	0.154 (3)
H34Q	0.362853	0.575704	0.512842	0.085*	0.154 (3)
H34R	0.390325	0.673309	0.485689	0.085*	0.154 (3)
N1B	0.7667 (3)	0.3243 (5)	0.2096 (3)	0.0223 (15)	
N2B	0.7794 (3)	0.1645 (5)	0.2095 (3)	0.0224 (15)	
N3B	0.5535 (3)	0.0389 (5)	0.3640 (3)	0.0190 (14)	
N4B	0.6096 (3)	0.1219 (5)	0.4286 (4)	0.0270 (16)	
C1B	0.7416 (4)	0.2388 (6)	0.2209 (4)	0.0203 (17)	
C2B	0.8237 (4)	0.3043 (6)	0.1898 (5)	0.0248 (19)	
C3B	0.8688 (4)	0.3664 (7)	0.1718 (5)	0.034 (2)	
H3BA	0.863281	0.434172	0.170396	0.041*	
C4B	0.9215 (4)	0.3251 (8)	0.1564 (6)	0.038 (2)	
H4BA	0.953081	0.365729	0.144579	0.046*	
C5B	0.9302 (4)	0.2248 (7)	0.1574 (5)	0.031 (2)	
H5BA	0.967241	0.199101	0.146059	0.038*	
C6B	0.8858 (4)	0.1637 (7)	0.1747 (4)	0.029 (2)	
H6BA	0.891536	0.095926	0.176091	0.035*	
C7B	0.8320 (4)	0.2045 (6)	0.1902 (4)	0.0211 (18)	
C8B	0.7685 (5)	0.0613 (6)	0.2132 (5)	0.035 (2)	
H8BA	0.729320	0.050636	0.231820	0.042*	
H8BB	0.797594	0.031982	0.242073	0.042*	
C9B	0.7715 (5)	0.0106 (7)	0.1499 (5)	0.044 (3)	
H9BA	0.804968	0.036029	0.125368	0.052*	
H9BB	0.735353	0.023709	0.125724	0.052*	
C10B	0.7786 (5)	-0.0982 (7)	0.1589 (5)	0.043 (2)	
H10C	0.812544	-0.110195	0.186870	0.051*	
H10D	0.743445	-0.123740	0.180306	0.051*	
C11B	0.7876 (6)	-0.1531 (9)	0.0970 (6)	0.055 (3)	
H11C	0.753890	-0.141305	0.068707	0.066*	
H11D	0.823116	-0.128590	0.075610	0.066*	
C12B	0.7939 (6)	-0.2601 (7)	0.1078 (6)	0.053 (3)	
H12D	0.799873	-0.292617	0.067156	0.079*	
H12E	0.758432	-0.285000	0.127923	0.079*	
H12F	0.827576	-0.272175	0.135354	0.079*	
C13B	0.6811 (3)	0.2286 (5)	0.2425 (4)	0.0191 (16)	
C14B	0.6381 (4)	0.2784 (6)	0.2093 (4)	0.0214 (17)	
H14B	0.648535	0.314712	0.172901	0.026*	
C15B	0.5796 (3)	0.2755 (5)	0.2288 (4)	0.0191 (17)	
C16B	0.5657 (3)	0.2196 (5)	0.2807 (4)	0.0190 (17)	
H16B	0.525957	0.214610	0.293345	0.023*	
C17B	0.6084 (4)	0.1701 (6)	0.3151 (4)	0.0194 (17)	
C18B	0.6664 (4)	0.1748 (6)	0.2958 (4)	0.0183 (16)	
H18B	0.695855	0.141562	0.318779	0.022*	

C19B	0.5324 (4)	0.3299 (6)	0.1905 (5)	0.029 (2)	
C20B	0.5184 (5)	0.2722 (7)	0.1314 (5)	0.037 (2)	
H20G	0.487844	0.305128	0.107264	0.056*	
H20H	0.504703	0.207876	0.143576	0.056*	
H20I	0.553625	0.266173	0.105375	0.056*	
C21B	0.5551 (4)	0.4300 (6)	0.1715 (5)	0.034 (2)	
H21G	0.523637	0.466529	0.151243	0.050*	
H21H	0.587766	0.422880	0.141859	0.050*	
H21I	0.568473	0.464423	0.209314	0.050*	
C22B	0.4769 (4)	0.3428 (7)	0.2295 (6)	0.037 (2)	
H22G	0.448756	0.381674	0.205605	0.056*	
H22H	0.486359	0.375425	0.269295	0.056*	
H22I	0.459799	0.279560	0.238631	0.056*	
C23B	0.5902 (3)	0.1098 (6)	0.3686 (4)	0.0199 (17)	
C24B	0.5475 (4)	0.0013 (6)	0.4250 (4)	0.0238 (18)	
C25B	0.5131 (6)	-0.0741 (9)	0.4486 (6)	0.055 (4)	
H25B	0.487665	-0.109470	0.421671	0.066*	
C26B	0.5173 (7)	-0.0950 (10)	0.5115 (6)	0.063 (4)	
H26B	0.496196	-0.148585	0.527625	0.075*	
C27B	0.5513 (5)	-0.0407 (8)	0.5533 (5)	0.042 (3)	
H27B	0.551430	-0.055549	0.597187	0.050*	
C28B	0.5844 (5)	0.0337 (8)	0.5310 (5)	0.036 (2)	
H28B	0.608254	0.070615	0.558637	0.044*	
C29B	0.5824 (4)	0.0539 (7)	0.4664 (4)	0.0251 (18)	
C30B	0.6566 (7)	0.1804 (14)	0.4558 (8)	0.033 (3)	0.622 (4)
H30C	0.642067	0.212093	0.494658	0.039*	0.622 (4)
H30D	0.667376	0.231478	0.425283	0.039*	0.622 (4)
C31B	0.7112 (6)	0.1213 (13)	0.4720 (8)	0.043 (3)	0.622 (4)
H31C	0.697765	0.064690	0.496501	0.051*	0.622 (4)
H31D	0.726833	0.096338	0.431544	0.051*	0.622 (4)
C32B	0.7619 (7)	0.1635 (13)	0.5075 (9)	0.051 (4)	0.622 (4)
H32C	0.748096	0.185528	0.549417	0.062*	0.622 (4)
H32D	0.776278	0.220603	0.484188	0.062*	0.622 (4)
C33B	0.8125 (8)	0.0937 (15)	0.5169 (11)	0.050 (5)	0.622 (4)
H33C	0.799466	0.038175	0.542684	0.060*	0.622 (4)
H33D	0.825893	0.069148	0.475425	0.060*	0.622 (4)
C34B	0.8615 (10)	0.144 (2)	0.5494 (12)	0.078 (6)	0.622 (4)
H34G	0.893156	0.097697	0.557276	0.117*	0.622 (4)
H34H	0.847678	0.169981	0.589724	0.117*	0.622 (4)
H34I	0.875849	0.196110	0.522596	0.117*	0.622 (4)
C30D	0.6324 (19)	0.225 (4)	0.455 (2)	0.031 (5)	0.224 (4)
H30G	0.651079	0.260090	0.419621	0.037*	0.224 (4)
H30H	0.598334	0.262677	0.469152	0.037*	0.224 (4)
C31D	0.6758 (14)	0.216 (3)	0.5091 (17)	0.036 (4)	0.224 (4)
H31G	0.661647	0.260357	0.542709	0.043*	0.224 (4)
H31H	0.671888	0.150242	0.526046	0.043*	0.224 (4)
C32D	0.7400 (14)	0.235 (3)	0.502 (2)	0.049 (5)	0.224 (4)
H32G	0.746583	0.305185	0.507051	0.059*	0.224 (4)

H32H	0.751535	0.217543	0.458631	0.059*	0.224 (4)
C33D	0.7810 (18)	0.183 (4)	0.548 (2)	0.053 (5)	0.224 (4)
H33G	0.802722	0.230970	0.573246	0.063*	0.224 (4)
H33H	0.757515	0.143207	0.577475	0.063*	0.224 (4)
C34D	0.823 (3)	0.120 (4)	0.514 (3)	0.052 (8)	0.224 (4)
H34J	0.838542	0.071261	0.543323	0.078*	0.224 (4)
H34K	0.855545	0.159038	0.497837	0.078*	0.224 (4)
H34L	0.803466	0.087831	0.478746	0.078*	0.224 (4)
C30E	0.642 (3)	0.213 (5)	0.443 (4)	0.032 (5)	0.154 (3)
H30I	0.660759	0.237768	0.404424	0.038*	0.154 (3)
H30J	0.672984	0.199656	0.474717	0.038*	0.154 (3)
C31E	0.601 (2)	0.290 (3)	0.470 (3)	0.032 (6)	0.154 (3)
H31I	0.576425	0.315794	0.434789	0.038*	0.154 (3)
H31J	0.573973	0.259743	0.500764	0.038*	0.154 (3)
C32E	0.631 (2)	0.374 (3)	0.502 (3)	0.036 (6)	0.154 (3)
H32I	0.663817	0.395621	0.474198	0.043*	0.154 (3)
H32J	0.648870	0.350630	0.541834	0.043*	0.154 (3)
C33E	0.592 (2)	0.461 (4)	0.516 (3)	0.048 (5)	0.154 (3)
H33I	0.574433	0.484567	0.476820	0.057*	0.154 (3)
H33J	0.560275	0.440285	0.545116	0.057*	0.154 (3)
C34E	0.626 (3)	0.540 (4)	0.547 (4)	0.053 (11)	0.154 (3)
H34M	0.664284	0.546349	0.525649	0.079*	0.154 (3)
H34N	0.632801	0.524443	0.591694	0.079*	0.154 (3)
H34O	0.604768	0.600389	0.543507	0.079*	0.154 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.02327 (15)	0.01836 (14)	0.0316 (2)	0.00293 (12)	0.00245 (14)	0.00065 (15)
Hg2	0.03127 (17)	0.02021 (14)	0.02125 (17)	-0.00420 (13)	-0.00170 (14)	-0.00320 (15)
Br12	0.0428 (6)	0.0365 (5)	0.0318 (5)	-0.0087 (4)	0.0078 (4)	-0.0070 (4)
Br22	0.0587 (7)	0.0351 (5)	0.0396 (6)	0.0027 (5)	0.0191 (5)	-0.0035 (4)
Br11	0.0125 (18)	0.0248 (11)	0.067 (2)	-0.0023 (11)	0.0074 (14)	0.0025 (10)
Br21	0.0360 (11)	0.019 (3)	0.029 (5)	-0.0054 (18)	-0.008 (4)	0.005 (3)
Cl11	0.0125 (18)	0.0248 (11)	0.067 (2)	-0.0023 (11)	0.0074 (14)	0.0025 (10)
Cl21	0.0360 (11)	0.019 (3)	0.029 (5)	-0.0054 (18)	-0.008 (4)	0.005 (3)
N1A	0.028 (4)	0.032 (4)	0.013 (3)	0.005 (3)	-0.005 (3)	-0.005 (3)
N2A	0.041 (4)	0.031 (4)	0.026 (4)	0.010 (3)	0.002 (3)	0.000 (3)
N3A	0.030 (4)	0.012 (3)	0.022 (4)	-0.005 (3)	-0.004 (3)	-0.001 (3)
N4A	0.050 (5)	0.019 (4)	0.034 (5)	-0.015 (3)	0.012 (4)	-0.007 (3)
C1A	0.030 (4)	0.020 (4)	0.015 (4)	0.000 (3)	0.002 (3)	-0.004 (3)
C2A	0.031 (7)	0.042 (7)	0.022 (6)	0.004 (6)	0.000 (6)	-0.006 (6)
C3A	0.036 (8)	0.049 (8)	0.024 (7)	0.007 (7)	0.002 (7)	-0.007 (7)
C4A	0.041 (8)	0.055 (8)	0.030 (7)	0.010 (8)	0.009 (7)	-0.010 (7)
C5A	0.044 (8)	0.059 (8)	0.026 (7)	0.003 (8)	0.007 (7)	-0.006 (7)
C6A	0.041 (8)	0.055 (8)	0.023 (7)	0.003 (7)	0.005 (7)	-0.002 (7)
C7A	0.037 (7)	0.045 (7)	0.023 (6)	0.004 (6)	0.002 (6)	-0.004 (6)
C2C	0.032 (5)	0.043 (6)	0.022 (5)	0.004 (4)	0.001 (4)	-0.006 (4)

C3C	0.036 (7)	0.047 (7)	0.025 (5)	0.006 (5)	0.005 (5)	-0.008 (5)
C4C	0.042 (7)	0.059 (7)	0.029 (5)	0.008 (7)	0.016 (5)	-0.009 (6)
C5C	0.044 (7)	0.066 (7)	0.022 (5)	0.008 (6)	0.011 (5)	-0.006 (5)
C6C	0.039 (7)	0.060 (7)	0.022 (5)	0.008 (6)	0.006 (5)	-0.004 (5)
C7C	0.035 (6)	0.047 (6)	0.025 (5)	0.006 (5)	0.005 (4)	-0.004 (5)
C8A	0.058 (7)	0.049 (6)	0.023 (5)	0.019 (5)	-0.002 (5)	0.008 (4)
C9A	0.037 (6)	0.097 (10)	0.039 (6)	0.025 (6)	0.012 (5)	0.022 (6)
C10A	0.085 (10)	0.123 (15)	0.059 (9)	0.067 (11)	-0.002 (8)	0.023 (9)
C11A	0.081 (11)	0.17 (2)	0.058 (10)	0.067 (12)	0.007 (8)	0.062 (12)
C12A	0.063 (9)	0.21 (2)	0.033 (8)	0.037 (12)	0.009 (7)	0.049 (11)
C13A	0.040 (5)	0.017 (4)	0.020 (4)	0.004 (4)	0.001 (4)	0.002 (3)
C14A	0.031 (4)	0.017 (3)	0.027 (5)	0.007 (3)	-0.002 (4)	0.000 (4)
C15A	0.042 (5)	0.017 (4)	0.026 (5)	0.003 (4)	-0.006 (4)	0.000 (3)
C16A	0.038 (5)	0.017 (4)	0.022 (5)	0.002 (4)	-0.002 (4)	-0.002 (3)
C17A	0.037 (5)	0.013 (4)	0.017 (4)	-0.004 (3)	0.002 (3)	0.002 (3)
C18A	0.039 (5)	0.015 (4)	0.011 (4)	0.002 (3)	0.002 (3)	-0.003 (3)
C19A	0.039 (5)	0.040 (5)	0.027 (5)	0.010 (4)	-0.015 (4)	-0.008 (4)
C20A	0.042 (10)	0.081 (13)	0.045 (10)	0.012 (10)	-0.024 (8)	-0.021 (10)
C21A	0.040 (9)	0.028 (9)	0.069 (12)	-0.002 (7)	-0.017 (9)	-0.011 (8)
C22A	0.082 (13)	0.075 (13)	0.032 (9)	-0.006 (11)	-0.031 (9)	0.001 (9)
C20C	0.067 (14)	0.058 (14)	0.045 (13)	-0.009 (12)	-0.020 (12)	0.002 (12)
C21C	0.060 (13)	0.063 (14)	0.060 (13)	0.014 (12)	-0.038 (11)	-0.020 (12)
C22C	0.037 (9)	0.058 (10)	0.030 (9)	0.010 (8)	-0.022 (8)	0.004 (8)
C23A	0.037 (5)	0.021 (4)	0.019 (4)	-0.010 (4)	0.006 (4)	-0.006 (3)
C24A	0.039 (5)	0.029 (5)	0.012 (4)	-0.012 (4)	0.004 (4)	-0.001 (3)
C25A	0.035 (5)	0.045 (6)	0.016 (4)	-0.001 (4)	-0.003 (4)	-0.006 (4)
C26A	0.032 (5)	0.054 (6)	0.023 (5)	-0.002 (5)	0.003 (4)	-0.015 (4)
C27A	0.046 (6)	0.059 (7)	0.017 (5)	-0.022 (5)	0.003 (4)	-0.007 (4)
C28A	0.047 (6)	0.037 (6)	0.036 (6)	-0.022 (5)	0.014 (5)	-0.003 (5)
C29A	0.051 (6)	0.029 (5)	0.025 (5)	-0.007 (5)	0.012 (4)	-0.013 (4)
C30A	0.066 (5)	0.024 (4)	0.051 (4)	-0.007 (4)	0.018 (4)	-0.001 (3)
C31A	0.068 (5)	0.028 (4)	0.047 (4)	-0.007 (4)	0.017 (4)	0.006 (4)
C32A	0.067 (5)	0.037 (4)	0.045 (5)	0.001 (4)	0.016 (4)	0.008 (4)
C33A	0.069 (7)	0.047 (7)	0.046 (6)	-0.002 (6)	0.009 (6)	0.006 (6)
C34A	0.068 (10)	0.079 (11)	0.059 (10)	0.007 (9)	0.007 (9)	0.018 (9)
C30C	0.066 (5)	0.024 (4)	0.051 (4)	-0.007 (4)	0.018 (4)	-0.001 (3)
C31C	0.068 (5)	0.028 (4)	0.047 (4)	-0.007 (4)	0.017 (4)	0.006 (4)
C32C	0.067 (5)	0.037 (4)	0.045 (5)	0.001 (4)	0.016 (4)	0.008 (4)
C33C	0.066 (8)	0.044 (8)	0.044 (7)	-0.002 (8)	0.014 (7)	0.008 (7)
C34C	0.061 (14)	0.058 (14)	0.042 (14)	0.002 (14)	0.014 (13)	0.014 (13)
C30F	0.066 (5)	0.024 (4)	0.051 (4)	-0.007 (4)	0.018 (4)	-0.001 (3)
C31F	0.068 (7)	0.031 (6)	0.051 (6)	-0.003 (6)	0.017 (6)	0.002 (6)
C32F	0.068 (7)	0.037 (6)	0.047 (6)	-0.003 (6)	0.014 (6)	0.007 (6)
C33F	0.071 (10)	0.035 (9)	0.047 (9)	-0.006 (9)	0.013 (9)	0.005 (9)
C34F	0.08 (3)	0.05 (3)	0.04 (2)	0.00 (3)	0.00 (2)	-0.01 (2)
N1B	0.026 (4)	0.012 (3)	0.029 (4)	0.009 (3)	0.007 (3)	-0.001 (3)
N2B	0.034 (4)	0.020 (3)	0.013 (3)	0.002 (3)	0.007 (3)	0.001 (3)
N3B	0.023 (3)	0.024 (3)	0.010 (3)	-0.007 (3)	-0.003 (3)	-0.002 (3)

N4B	0.031 (4)	0.028 (4)	0.021 (4)	-0.006 (3)	-0.004 (3)	-0.002 (3)
C1B	0.029 (4)	0.017 (4)	0.015 (4)	0.002 (3)	0.002 (3)	0.001 (3)
C2B	0.023 (4)	0.017 (4)	0.035 (5)	0.003 (3)	0.008 (4)	-0.006 (4)
C3B	0.033 (5)	0.017 (4)	0.052 (6)	-0.002 (4)	0.007 (5)	0.002 (4)
C4B	0.029 (5)	0.036 (5)	0.050 (6)	-0.002 (4)	0.013 (5)	-0.001 (5)
C5B	0.029 (5)	0.038 (5)	0.027 (5)	0.014 (4)	0.009 (4)	0.002 (4)
C6B	0.039 (5)	0.030 (5)	0.020 (4)	0.016 (4)	0.012 (4)	0.006 (4)
C7B	0.029 (5)	0.020 (4)	0.014 (4)	0.003 (4)	0.005 (3)	0.002 (3)
C8B	0.044 (6)	0.017 (4)	0.044 (6)	0.003 (4)	0.021 (4)	-0.003 (4)
C9B	0.056 (7)	0.041 (6)	0.034 (6)	-0.009 (5)	0.011 (5)	-0.009 (5)
C10B	0.049 (6)	0.039 (6)	0.040 (6)	-0.006 (5)	0.007 (5)	-0.001 (5)
C11B	0.054 (7)	0.054 (7)	0.056 (7)	-0.008 (6)	0.011 (6)	-0.014 (6)
C12B	0.081 (9)	0.027 (5)	0.051 (7)	0.022 (6)	-0.021 (6)	-0.023 (5)
C13B	0.023 (4)	0.016 (3)	0.019 (4)	0.000 (3)	0.003 (3)	-0.006 (3)
C14B	0.025 (4)	0.014 (4)	0.025 (5)	-0.001 (3)	0.001 (3)	-0.001 (3)
C15B	0.022 (4)	0.011 (4)	0.024 (4)	-0.001 (3)	-0.010 (3)	-0.006 (3)
C16B	0.015 (3)	0.014 (4)	0.027 (5)	0.002 (3)	0.001 (3)	-0.007 (3)
C17B	0.023 (4)	0.020 (4)	0.016 (4)	-0.001 (3)	-0.003 (3)	-0.009 (3)
C18B	0.025 (4)	0.011 (4)	0.019 (4)	-0.001 (3)	-0.001 (3)	-0.002 (3)
C19B	0.030 (5)	0.020 (4)	0.036 (5)	-0.001 (4)	-0.008 (4)	0.004 (4)
C20B	0.048 (6)	0.029 (5)	0.035 (5)	0.001 (4)	-0.021 (5)	0.001 (4)
C21B	0.037 (5)	0.018 (4)	0.045 (6)	0.001 (4)	-0.006 (4)	0.009 (4)
C22B	0.024 (5)	0.023 (4)	0.065 (7)	0.005 (4)	-0.003 (4)	0.005 (4)
C23B	0.020 (4)	0.021 (4)	0.019 (4)	0.002 (3)	0.003 (3)	-0.001 (3)
C24B	0.033 (5)	0.028 (4)	0.010 (4)	-0.003 (4)	-0.003 (3)	-0.002 (3)
C25B	0.093 (10)	0.045 (7)	0.027 (6)	-0.039 (7)	0.007 (6)	0.002 (5)
C26B	0.098 (11)	0.068 (9)	0.021 (5)	-0.048 (8)	0.005 (6)	0.002 (5)
C27B	0.062 (7)	0.051 (6)	0.012 (4)	-0.008 (5)	-0.007 (4)	0.000 (4)
C28B	0.042 (5)	0.043 (6)	0.024 (5)	-0.006 (5)	-0.012 (4)	-0.004 (4)
C29B	0.025 (4)	0.032 (5)	0.018 (4)	0.003 (4)	0.003 (3)	0.001 (4)
C30B	0.031 (7)	0.046 (8)	0.022 (6)	-0.014 (6)	0.000 (6)	-0.002 (6)
C31B	0.037 (7)	0.059 (8)	0.032 (6)	-0.008 (6)	0.008 (5)	0.019 (6)
C32B	0.066 (8)	0.049 (7)	0.040 (7)	-0.007 (7)	0.017 (6)	0.014 (7)
C33B	0.064 (9)	0.054 (9)	0.032 (7)	-0.004 (8)	0.014 (7)	0.012 (8)
C34B	0.083 (13)	0.085 (13)	0.066 (12)	-0.017 (12)	0.003 (11)	0.013 (11)
C30D	0.034 (10)	0.040 (10)	0.018 (9)	-0.011 (9)	-0.005 (9)	-0.002 (9)
C31D	0.038 (9)	0.047 (9)	0.024 (8)	-0.009 (8)	0.001 (8)	0.006 (8)
C32D	0.054 (9)	0.055 (9)	0.038 (8)	-0.007 (8)	0.009 (8)	0.013 (9)
C33D	0.063 (10)	0.055 (10)	0.041 (9)	-0.004 (9)	0.009 (9)	0.014 (9)
C34D	0.062 (15)	0.059 (16)	0.035 (14)	-0.011 (15)	0.016 (14)	0.016 (14)
C30E	0.034 (10)	0.042 (11)	0.019 (10)	-0.010 (9)	-0.002 (9)	-0.001 (9)
C31E	0.036 (11)	0.040 (11)	0.019 (11)	-0.006 (10)	0.006 (10)	-0.002 (10)
C32E	0.043 (12)	0.040 (12)	0.025 (11)	-0.004 (12)	0.011 (11)	0.006 (11)
C33E	0.058 (10)	0.049 (9)	0.037 (9)	-0.004 (9)	0.011 (9)	0.004 (9)
C34E	0.06 (2)	0.05 (2)	0.04 (2)	0.00 (2)	0.003 (19)	0.008 (19)

Geometric parameters (Å, °)

Hg1—N1A	2.313 (7)	C34C—H34E	0.9800
Hg1—N1B	2.343 (6)	C34C—H34F	0.9800
Hg1—C111	2.373 (19)	C30F—C31F	1.53 (3)
Hg1—Br12	2.5083 (10)	C30F—H30K	0.9900
Hg1—Br11	2.593 (4)	C30F—H30L	0.9900
Hg2—N3A ⁱ	2.316 (6)	C31F—C32F	1.52 (3)
Hg2—N3B	2.327 (6)	C31F—H31K	0.9900
Hg2—C121	2.48 (4)	C31F—H31L	0.9900
Hg2—Br22	2.5147 (11)	C32F—C33F	1.53 (3)
Hg2—Br21	2.57 (2)	C32F—H32K	0.9900
N1A—C1A	1.326 (11)	C32F—H32L	0.9900
N1A—C2A	1.39 (2)	C33F—C34F	1.50 (3)
N1A—C2C	1.408 (15)	C33F—H33K	0.9900
N2A—C1A	1.364 (12)	C33F—H33L	0.9900
N2A—C7A	1.38 (2)	C34F—H34P	0.9800
N2A—C7C	1.384 (15)	C34F—H34Q	0.9800
N2A—C8A	1.460 (13)	C34F—H34R	0.9800
N3A—C23A	1.324 (11)	N1B—C1B	1.340 (11)
N3A—C24A	1.391 (12)	N1B—C2B	1.398 (11)
N4A—C23A	1.372 (12)	N2B—C1B	1.368 (11)
N4A—C29A	1.376 (14)	N2B—C7B	1.388 (11)
N4A—C30F	1.461 (13)	N2B—C8B	1.456 (11)
N4A—C30A	1.461 (13)	N3B—C23B	1.300 (11)
N4A—C30C	1.461 (13)	N3B—C24B	1.396 (12)
C1A—C13A	1.466 (12)	N4B—C23B	1.354 (11)
C2A—C7A	1.38 (3)	N4B—C29B	1.385 (12)
C2A—C3A	1.39 (3)	N4B—C30B	1.465 (17)
C3A—C4A	1.41 (3)	N4B—C30E	1.50 (7)
C3A—H3AA	0.9500	N4B—C30D	1.62 (5)
C4A—C5A	1.36 (3)	C1B—C13B	1.464 (11)
C4A—H4AA	0.9500	C2B—C3B	1.397 (13)
C5A—C6A	1.37 (3)	C2B—C7B	1.400 (12)
C5A—H5AA	0.9500	C3B—C4B	1.375 (14)
C6A—C7A	1.40 (3)	C3B—H3BA	0.9500
C6A—H6AA	0.9500	C4B—C5B	1.407 (14)
C2C—C7C	1.387 (17)	C4B—H4BA	0.9500
C2C—C3C	1.402 (17)	C5B—C6B	1.375 (14)
C3C—C4C	1.40 (2)	C5B—H5BA	0.9500
C3C—H3CA	0.9500	C6B—C7B	1.394 (12)
C4C—C5C	1.36 (2)	C6B—H6BA	0.9500
C4C—H4CA	0.9500	C8B—C9B	1.513 (13)
C5C—C6C	1.374 (19)	C8B—H8BA	0.9900
C5C—H5CA	0.9500	C8B—H8BB	0.9900
C6C—C7C	1.398 (16)	C9B—C10B	1.532 (14)
C6C—H6CA	0.9500	C9B—H9BA	0.9900
C8A—C9A	1.497 (17)	C9B—H9BB	0.9900

C8A—H8AA	0.9900	C10B—C11B	1.528 (14)
C8A—H8AB	0.9900	C10B—H10C	0.9900
C9A—C10A	1.52 (2)	C10B—H10D	0.9900
C9A—H9A1	0.9900	C11B—C12B	1.510 (15)
C9A—H9A2	0.9900	C11B—H11C	0.9900
C10A—C11A	1.53 (2)	C11B—H11D	0.9900
C10A—H10A	0.9900	C12B—H12D	0.9800
C10A—H10B	0.9900	C12B—H12E	0.9800
C11A—C12A	1.49 (3)	C12B—H12F	0.9800
C11A—H11A	0.9900	C13B—C14B	1.392 (12)
C11A—H11B	0.9900	C13B—C18B	1.393 (12)
C12A—H12A	0.9800	C14B—C15B	1.401 (12)
C12A—H12B	0.9800	C14B—H14B	0.9500
C12A—H12C	0.9800	C15B—C16B	1.380 (12)
C13A—C18A	1.391 (13)	C15B—C19B	1.547 (11)
C13A—C14A	1.406 (13)	C16B—C17B	1.401 (12)
C14A—C15A	1.400 (13)	C16B—H16B	0.9500
C14A—H14A	0.9500	C17B—C18B	1.390 (12)
C15A—C16A	1.383 (14)	C17B—C23B	1.467 (12)
C15A—C19A	1.532 (13)	C18B—H18B	0.9500
C16A—C17A	1.383 (13)	C19B—C20B	1.518 (14)
C16A—H16A	0.9500	C19B—C22B	1.526 (14)
C17A—C18A	1.395 (11)	C19B—C21B	1.537 (12)
C17A—C23A	1.466 (13)	C20B—H20G	0.9800
C18A—H18A	0.9500	C20B—H20H	0.9800
C19A—C20C	1.43 (4)	C20B—H20I	0.9800
C19A—C22A	1.47 (3)	C21B—H21G	0.9800
C19A—C21C	1.54 (3)	C21B—H21H	0.9800
C19A—C20A	1.54 (2)	C21B—H21I	0.9800
C19A—C21A	1.55 (2)	C22B—H22G	0.9800
C19A—C22C	1.58 (3)	C22B—H22H	0.9800
C20A—H20A	0.9800	C22B—H22I	0.9800
C20A—H20B	0.9800	C24B—C29B	1.391 (13)
C20A—H20C	0.9800	C24B—C25B	1.402 (14)
C21A—H21A	0.9800	C25B—C26B	1.366 (17)
C21A—H21B	0.9800	C25B—H25B	0.9500
C21A—H21C	0.9800	C26B—C27B	1.398 (16)
C22A—H22A	0.9800	C26B—H26B	0.9500
C22A—H22B	0.9800	C27B—C28B	1.365 (16)
C22A—H22C	0.9800	C27B—H27B	0.9500
C20C—H20D	0.9800	C28B—C29B	1.395 (13)
C20C—H20E	0.9800	C28B—H28B	0.9500
C20C—H20F	0.9800	C30B—C31B	1.534 (19)
C21C—H21D	0.9800	C30B—H30C	0.9900
C21C—H21E	0.9800	C30B—H30D	0.9900
C21C—H21F	0.9800	C31B—C32B	1.500 (19)
C22C—H22D	0.9800	C31B—H31C	0.9900
C22C—H22E	0.9800	C31B—H31D	0.9900

C22C—H22F	0.9800	C32B—C33B	1.52 (2)
C24A—C29A	1.390 (13)	C32B—H32C	0.9900
C24A—C25A	1.406 (14)	C32B—H32D	0.9900
C25A—C26A	1.378 (14)	C33B—C34B	1.48 (2)
C25A—H25A	0.9500	C33B—H33C	0.9900
C26A—C27A	1.385 (16)	C33B—H33D	0.9900
C26A—H26A	0.9500	C34B—H34G	0.9800
C27A—C28A	1.358 (17)	C34B—H34H	0.9800
C27A—H27A	0.9500	C34B—H34I	0.9800
C28A—C29A	1.415 (14)	C30D—C31D	1.52 (2)
C28A—H28A	0.9500	C30D—H30G	0.9900
C30A—C31A	1.559 (15)	C30D—H30H	0.9900
C30A—H30A	0.9900	C31D—C32D	1.50 (2)
C30A—H30B	0.9900	C31D—H31G	0.9900
C31A—C32A	1.519 (17)	C31D—H31H	0.9900
C31A—H31A	0.9900	C32D—C33D	1.53 (3)
C31A—H31B	0.9900	C32D—H32G	0.9900
C32A—C33A	1.544 (18)	C32D—H32H	0.9900
C32A—H32A	0.9900	C33D—C34D	1.49 (3)
C32A—H32B	0.9900	C33D—H33G	0.9900
C33A—C34A	1.51 (2)	C33D—H33H	0.9900
C33A—H33A	0.9900	C34D—H34J	0.9800
C33A—H33B	0.9900	C34D—H34K	0.9800
C34A—H34A	0.9800	C34D—H34L	0.9800
C34A—H34B	0.9800	C30E—C31E	1.53 (3)
C34A—H34C	0.9800	C30E—H30I	0.9900
C30C—C31C	1.559 (15)	C30E—H30J	0.9900
C30C—H30E	0.9900	C31E—C32E	1.52 (3)
C30C—H30F	0.9900	C31E—H31I	0.9900
C31C—C32C	1.519 (17)	C31E—H31J	0.9900
C31C—H31E	0.9900	C32E—C33E	1.53 (3)
C31C—H31F	0.9900	C32E—H32I	0.9900
C32C—C33C	1.53 (3)	C32E—H32J	0.9900
C32C—H32E	0.9900	C33E—C34E	1.50 (3)
C32C—H32F	0.9900	C33E—H33I	0.9900
C33C—C34C	1.50 (3)	C33E—H33J	0.9900
C33C—H33E	0.9900	C34E—H34M	0.9800
C33C—H33F	0.9900	C34E—H34N	0.9800
C34C—H34D	0.9800	C34E—H34O	0.9800
N1A—Hg1—N1B	99.4 (3)	H34D—C34C—H34F	109.5
N1A—Hg1—Cl11	107.1 (6)	H34E—C34C—H34F	109.5
N1B—Hg1—Cl11	108.0 (5)	N4A—C30F—C31F	110 (3)
N1A—Hg1—Br12	115.82 (18)	N4A—C30F—H30K	109.6
N1B—Hg1—Br12	111.26 (17)	C31F—C30F—H30K	109.6
Cl11—Hg1—Br12	114.1 (5)	N4A—C30F—H30L	109.6
N1A—Hg1—Br11	103.9 (2)	C31F—C30F—H30L	109.6
N1B—Hg1—Br11	105.2 (2)	H30K—C30F—H30L	108.2

Br12—Hg1—Br11	119.01 (12)	C32F—C31F—C30F	112 (3)
N3A ⁱ —Hg2—N3B	97.2 (2)	C32F—C31F—H31K	109.3
N3A ⁱ —Hg2—Cl21	101.7 (8)	C30F—C31F—H31K	109.3
N3B—Hg2—Cl21	105.0 (9)	C32F—C31F—H31L	109.3
N3A ⁱ —Hg2—Br22	115.13 (18)	C30F—C31F—H31L	109.3
N3B—Hg2—Br22	109.95 (17)	H31K—C31F—H31L	108.0
Cl21—Hg2—Br22	124.1 (7)	C31F—C32F—C33F	110 (3)
N3A ⁱ —Hg2—Br21	105.3 (5)	C31F—C32F—H32K	109.6
N3B—Hg2—Br21	107.8 (5)	C33F—C32F—H32K	109.6
Br22—Hg2—Br21	119.1 (4)	C31F—C32F—H32L	109.6
C1A—N1A—C2A	106 (2)	C33F—C32F—H32L	109.6
C1A—N1A—C2C	105.2 (10)	H32K—C32F—H32L	108.1
C1A—N1A—Hg1	124.8 (6)	C34F—C33F—C32F	110 (3)
C2A—N1A—Hg1	129 (2)	C34F—C33F—H33K	109.6
C2C—N1A—Hg1	129.4 (9)	C32F—C33F—H33K	109.6
C1A—N2A—C7A	106 (2)	C34F—C33F—H33L	109.6
C1A—N2A—C7C	108.1 (11)	C32F—C33F—H33L	109.6
C1A—N2A—C8A	127.7 (8)	H33K—C33F—H33L	108.2
C7A—N2A—C8A	126 (2)	C33F—C34F—H34P	109.5
C7C—N2A—C8A	123.0 (11)	C33F—C34F—H34Q	109.5
C23A—N3A—C24A	106.5 (7)	H34P—C34F—H34Q	109.5
C23A—N3A—Hg2 ⁱⁱ	125.9 (6)	C33F—C34F—H34R	109.5
C24A—N3A—Hg2 ⁱⁱ	125.5 (6)	H34P—C34F—H34R	109.5
C23A—N4A—C29A	107.0 (8)	H34Q—C34F—H34R	109.5
C23A—N4A—C30F	127.6 (9)	C1B—N1B—C2B	106.2 (7)
C29A—N4A—C30F	125.0 (8)	C1B—N1B—Hg1	124.8 (5)
C23A—N4A—C30A	127.6 (9)	C2B—N1B—Hg1	124.7 (5)
C29A—N4A—C30A	125.0 (8)	C1B—N2B—C7B	107.4 (7)
C23A—N4A—C30C	127.6 (9)	C1B—N2B—C8B	128.6 (8)
C29A—N4A—C30C	125.0 (8)	C7B—N2B—C8B	123.9 (7)
N1A—C1A—N2A	111.6 (7)	C23B—N3B—C24B	106.1 (7)
N1A—C1A—C13A	124.8 (8)	C23B—N3B—Hg2	123.6 (5)
N2A—C1A—C13A	123.5 (8)	C24B—N3B—Hg2	129.7 (5)
C7A—C2A—N1A	108 (3)	C23B—N4B—C29B	108.0 (7)
C7A—C2A—C3A	123 (2)	C23B—N4B—C30B	132.5 (9)
N1A—C2A—C3A	129 (4)	C29B—N4B—C30B	118.8 (9)
C2A—C3A—C4A	116 (3)	C23B—N4B—C30E	117 (3)
C2A—C3A—H3AA	122.1	C29B—N4B—C30E	133 (3)
C4A—C3A—H3AA	122.1	C23B—N4B—C30D	122.4 (17)
C5A—C4A—C3A	120 (3)	C29B—N4B—C30D	123.3 (19)
C5A—C4A—H4AA	120.0	N1B—C1B—N2B	111.4 (7)
C3A—C4A—H4AA	120.0	N1B—C1B—C13B	123.1 (7)
C4A—C5A—C6A	125 (3)	N2B—C1B—C13B	125.5 (7)
C4A—C5A—H5AA	117.3	C3B—C2B—N1B	130.5 (8)
C6A—C5A—H5AA	117.3	C3B—C2B—C7B	120.8 (8)
C5A—C6A—C7A	115 (3)	N1B—C2B—C7B	108.8 (7)
C5A—C6A—H6AA	122.5	C4B—C3B—C2B	117.1 (9)
C7A—C6A—H6AA	122.5	C4B—C3B—H3BA	121.4

N2A—C7A—C2A	107 (3)	C2B—C3B—H3BA	121.4
N2A—C7A—C6A	131 (4)	C3B—C4B—C5B	122.2 (9)
C2A—C7A—C6A	121 (2)	C3B—C4B—H4BA	118.9
C7C—C2C—C3C	118.4 (12)	C5B—C4B—H4BA	118.9
C7C—C2C—N1A	109.6 (14)	C6B—C5B—C4B	120.7 (9)
C3C—C2C—N1A	132.0 (15)	C6B—C5B—H5BA	119.7
C4C—C3C—C2C	118.4 (13)	C4B—C5B—H5BA	119.7
C4C—C3C—H3CA	120.8	C5B—C6B—C7B	117.7 (8)
C2C—C3C—H3CA	120.8	C5B—C6B—H6BA	121.1
C5C—C4C—C3C	121.4 (13)	C7B—C6B—H6BA	121.1
C5C—C4C—H4CA	119.3	N2B—C7B—C6B	132.3 (8)
C3C—C4C—H4CA	119.3	N2B—C7B—C2B	106.2 (7)
C4C—C5C—C6C	121.7 (13)	C6B—C7B—C2B	121.4 (8)
C4C—C5C—H5CA	119.2	N2B—C8B—C9B	113.6 (8)
C6C—C5C—H5CA	119.2	N2B—C8B—H8BA	108.8
C5C—C6C—C7C	117.1 (13)	C9B—C8B—H8BA	108.8
C5C—C6C—H6CA	121.5	N2B—C8B—H8BB	108.8
C7C—C6C—H6CA	121.5	C9B—C8B—H8BB	108.8
N2A—C7C—C2C	105.3 (14)	H8BA—C8B—H8BB	107.7
N2A—C7C—C6C	131.7 (16)	C8B—C9B—C10B	110.7 (9)
C2C—C7C—C6C	122.9 (12)	C8B—C9B—H9BA	109.5
N2A—C8A—C9A	113.0 (11)	C10B—C9B—H9BA	109.5
N2A—C8A—H8AA	109.0	C8B—C9B—H9BB	109.5
C9A—C8A—H8AA	109.0	C10B—C9B—H9BB	109.5
N2A—C8A—H8AB	109.0	H9BA—C9B—H9BB	108.1
C9A—C8A—H8AB	109.0	C11B—C10B—C9B	113.6 (9)
H8AA—C8A—H8AB	107.8	C11B—C10B—H10C	108.8
C8A—C9A—C10A	111.0 (14)	C9B—C10B—H10C	108.8
C8A—C9A—H9A1	109.4	C11B—C10B—H10D	108.8
C10A—C9A—H9A1	109.4	C9B—C10B—H10D	108.8
C8A—C9A—H9A2	109.4	H10C—C10B—H10D	107.7
C10A—C9A—H9A2	109.4	C12B—C11B—C10B	112.0 (10)
H9A1—C9A—H9A2	108.0	C12B—C11B—H11C	109.2
C9A—C10A—C11A	114.3 (12)	C10B—C11B—H11C	109.2
C9A—C10A—H10A	108.7	C12B—C11B—H11D	109.2
C11A—C10A—H10A	108.7	C10B—C11B—H11D	109.2
C9A—C10A—H10B	108.7	H11C—C11B—H11D	107.9
C11A—C10A—H10B	108.7	C11B—C12B—H12D	109.5
H10A—C10A—H10B	107.6	C11B—C12B—H12E	109.5
C12A—C11A—C10A	115.5 (18)	H12D—C12B—H12E	109.5
C12A—C11A—H11A	108.4	C11B—C12B—H12F	109.5
C10A—C11A—H11A	108.4	H12D—C12B—H12F	109.5
C12A—C11A—H11B	108.4	H12E—C12B—H12F	109.5
C10A—C11A—H11B	108.4	C14B—C13B—C18B	120.3 (8)
H11A—C11A—H11B	107.5	C14B—C13B—C1B	117.6 (7)
C11A—C12A—H12A	109.5	C18B—C13B—C1B	122.1 (7)
C11A—C12A—H12B	109.5	C13B—C14B—C15B	120.8 (8)
H12A—C12A—H12B	109.5	C13B—C14B—H14B	119.6

C11A—C12A—H12C	109.5	C15B—C14B—H14B	119.6
H12A—C12A—H12C	109.5	C16B—C15B—C14B	118.1 (7)
H12B—C12A—H12C	109.5	C16B—C15B—C19B	121.9 (7)
C18A—C13A—C14A	119.6 (8)	C14B—C15B—C19B	119.9 (8)
C18A—C13A—C1A	121.0 (8)	C15B—C16B—C17B	121.8 (7)
C14A—C13A—C1A	119.4 (8)	C15B—C16B—H16B	119.1
C15A—C14A—C13A	121.0 (8)	C17B—C16B—H16B	119.1
C15A—C14A—H14A	119.5	C18B—C17B—C16B	119.4 (8)
C13A—C14A—H14A	119.5	C18B—C17B—C23B	121.6 (8)
C16A—C15A—C14A	117.6 (8)	C16B—C17B—C23B	118.8 (7)
C16A—C15A—C19A	120.3 (8)	C17B—C18B—C13B	119.5 (8)
C14A—C15A—C19A	122.0 (9)	C17B—C18B—H18B	120.2
C17A—C16A—C15A	122.5 (9)	C13B—C18B—H18B	120.2
C17A—C16A—H16A	118.8	C20B—C19B—C22B	109.3 (8)
C15A—C16A—H16A	118.8	C20B—C19B—C21B	109.5 (8)
C16A—C17A—C18A	119.6 (9)	C22B—C19B—C21B	108.4 (8)
C16A—C17A—C23A	118.6 (8)	C20B—C19B—C15B	108.7 (7)
C18A—C17A—C23A	121.8 (8)	C22B—C19B—C15B	110.9 (8)
C13A—C18A—C17A	119.6 (8)	C21B—C19B—C15B	110.0 (7)
C13A—C18A—H18A	120.2	C19B—C20B—H20G	109.5
C17A—C18A—H18A	120.2	C19B—C20B—H20H	109.5
C20C—C19A—C15A	111.3 (15)	H20G—C20B—H20H	109.5
C22A—C19A—C15A	110.8 (12)	C19B—C20B—H20I	109.5
C20C—C19A—C21C	117 (2)	H20G—C20B—H20I	109.5
C15A—C19A—C21C	109.6 (13)	H20H—C20B—H20I	109.5
C22A—C19A—C20A	108.3 (16)	C19B—C21B—H21G	109.5
C15A—C19A—C20A	114.6 (11)	C19B—C21B—H21H	109.5
C22A—C19A—C21A	107.8 (16)	H21G—C21B—H21H	109.5
C15A—C19A—C21A	109.7 (10)	C19B—C21B—H21I	109.5
C20A—C19A—C21A	105.4 (15)	H21G—C21B—H21I	109.5
C20C—C19A—C22C	109.7 (19)	H21H—C21B—H21I	109.5
C15A—C19A—C22C	105.0 (12)	C19B—C22B—H22G	109.5
C21C—C19A—C22C	103.8 (18)	C19B—C22B—H22H	109.5
C19A—C20A—H20A	109.5	H22G—C22B—H22H	109.5
C19A—C20A—H20B	109.5	C19B—C22B—H22I	109.5
H20A—C20A—H20B	109.5	H22G—C22B—H22I	109.5
C19A—C20A—H20C	109.5	H22H—C22B—H22I	109.5
H20A—C20A—H20C	109.5	N3B—C23B—N4B	112.1 (7)
H20B—C20A—H20C	109.5	N3B—C23B—C17B	124.0 (7)
C19A—C21A—H21A	109.5	N4B—C23B—C17B	124.0 (7)
C19A—C21A—H21B	109.5	C29B—C24B—N3B	109.2 (8)
H21A—C21A—H21B	109.5	C29B—C24B—C25B	119.3 (9)
C19A—C21A—H21C	109.5	N3B—C24B—C25B	131.5 (9)
H21A—C21A—H21C	109.5	C26B—C25B—C24B	117.8 (11)
H21B—C21A—H21C	109.5	C26B—C25B—H25B	121.1
C19A—C22A—H22A	109.5	C24B—C25B—H25B	121.1
C19A—C22A—H22B	109.5	C25B—C26B—C27B	122.7 (11)
H22A—C22A—H22B	109.5	C25B—C26B—H26B	118.6

C19A—C22A—H22C	109.5	C27B—C26B—H26B	118.6
H22A—C22A—H22C	109.5	C28B—C27B—C26B	119.9 (10)
H22B—C22A—H22C	109.5	C28B—C27B—H27B	120.1
C19A—C20C—H20D	109.5	C26B—C27B—H27B	120.1
C19A—C20C—H20E	109.5	C27B—C28B—C29B	118.2 (9)
H20D—C20C—H20E	109.5	C27B—C28B—H28B	120.9
C19A—C20C—H20F	109.5	C29B—C28B—H28B	120.9
H20D—C20C—H20F	109.5	N4B—C29B—C24B	104.6 (8)
H20E—C20C—H20F	109.5	N4B—C29B—C28B	133.3 (9)
C19A—C21C—H21D	109.5	C24B—C29B—C28B	122.0 (9)
C19A—C21C—H21E	109.5	N4B—C30B—C31B	113.0 (14)
H21D—C21C—H21E	109.5	N4B—C30B—H30C	109.0
C19A—C21C—H21F	109.5	C31B—C30B—H30C	109.0
H21D—C21C—H21F	109.5	N4B—C30B—H30D	109.0
H21E—C21C—H21F	109.5	C31B—C30B—H30D	109.0
C19A—C22C—H22D	109.5	H30C—C30B—H30D	107.8
C19A—C22C—H22E	109.5	C32B—C31B—C30B	122.3 (15)
H22D—C22C—H22E	109.5	C32B—C31B—H31C	106.8
C19A—C22C—H22F	109.5	C30B—C31B—H31C	106.8
H22D—C22C—H22F	109.5	C32B—C31B—H31D	106.8
H22E—C22C—H22F	109.5	C30B—C31B—H31D	106.8
N3A—C23A—N4A	111.3 (8)	H31C—C31B—H31D	106.6
N3A—C23A—C17A	123.7 (8)	C31B—C32B—C33B	114.0 (15)
N4A—C23A—C17A	124.9 (8)	C31B—C32B—H32C	108.8
C29A—C24A—N3A	108.5 (9)	C33B—C32B—H32C	108.8
C29A—C24A—C25A	120.0 (9)	C31B—C32B—H32D	108.8
N3A—C24A—C25A	131.4 (8)	C33B—C32B—H32D	108.8
C26A—C25A—C24A	116.9 (10)	H32C—C32B—H32D	107.7
C26A—C25A—H25A	121.5	C34B—C33B—C32B	109.8 (18)
C24A—C25A—H25A	121.5	C34B—C33B—H33C	109.7
C25A—C26A—C27A	121.8 (10)	C32B—C33B—H33C	109.7
C25A—C26A—H26A	119.1	C34B—C33B—H33D	109.7
C27A—C26A—H26A	119.1	C32B—C33B—H33D	109.7
C28A—C27A—C26A	123.3 (10)	H33C—C33B—H33D	108.2
C28A—C27A—H27A	118.4	C33B—C34B—H34G	109.5
C26A—C27A—H27A	118.4	C33B—C34B—H34H	109.5
C27A—C28A—C29A	115.3 (9)	H34G—C34B—H34H	109.5
C27A—C28A—H28A	122.4	C33B—C34B—H34I	109.5
C29A—C28A—H28A	122.4	H34G—C34B—H34I	109.5
N4A—C29A—C24A	106.6 (9)	H34H—C34B—H34I	109.5
N4A—C29A—C28A	130.7 (9)	C31D—C30D—N4B	114 (4)
C24A—C29A—C28A	122.7 (10)	C31D—C30D—H30G	108.8
N4A—C30A—C31A	112.8 (9)	N4B—C30D—H30G	108.8
N4A—C30A—H30A	109.0	C31D—C30D—H30H	108.8
C31A—C30A—H30A	109.0	N4B—C30D—H30H	108.8
N4A—C30A—H30B	109.0	H30G—C30D—H30H	107.7
C31A—C30A—H30B	109.0	C32D—C31D—C30D	124 (3)
H30A—C30A—H30B	107.8	C32D—C31D—H31G	106.4

C32A—C31A—C30A	115.4 (10)	C30D—C31D—H31G	106.4
C32A—C31A—H31A	108.4	C32D—C31D—H31H	106.4
C30A—C31A—H31A	108.4	C30D—C31D—H31H	106.4
C32A—C31A—H31B	108.4	H31G—C31D—H31H	106.5
C30A—C31A—H31B	108.4	C31D—C32D—C33D	117 (3)
H31A—C31A—H31B	107.5	C31D—C32D—H32G	108.0
C31A—C32A—C33A	111.6 (11)	C33D—C32D—H32G	108.0
C31A—C32A—H32A	109.3	C31D—C32D—H32H	108.0
C33A—C32A—H32A	109.3	C33D—C32D—H32H	108.0
C31A—C32A—H32B	109.3	H32G—C32D—H32H	107.2
C33A—C32A—H32B	109.3	C34D—C33D—C32D	112 (3)
H32A—C32A—H32B	108.0	C34D—C33D—H33G	109.2
C34A—C33A—C32A	109.9 (14)	C32D—C33D—H33G	109.2
C34A—C33A—H33A	109.7	C34D—C33D—H33H	109.2
C32A—C33A—H33A	109.7	C32D—C33D—H33H	109.2
C34A—C33A—H33B	109.7	H33G—C33D—H33H	107.9
C32A—C33A—H33B	109.7	C33D—C34D—H34J	109.5
H33A—C33A—H33B	108.2	C33D—C34D—H34K	109.5
C33A—C34A—H34A	109.5	H34J—C34D—H34K	109.5
C33A—C34A—H34B	109.5	C33D—C34D—H34L	109.5
H34A—C34A—H34B	109.5	H34J—C34D—H34L	109.5
C33A—C34A—H34C	109.5	H34K—C34D—H34L	109.5
H34A—C34A—H34C	109.5	N4B—C30E—C31E	111 (5)
H34B—C34A—H34C	109.5	N4B—C30E—H30I	109.4
N4A—C30C—C31C	112.8 (9)	C31E—C30E—H30I	109.4
N4A—C30C—H30E	109.0	N4B—C30E—H30J	109.4
C31C—C30C—H30E	109.0	C31E—C30E—H30J	109.4
N4A—C30C—H30F	109.0	H30I—C30E—H30J	108.0
C31C—C30C—H30F	109.0	C32E—C31E—C30E	114 (3)
H30E—C30C—H30F	107.8	C32E—C31E—H31I	108.7
C32C—C31C—C30C	115.4 (10)	C30E—C31E—H31I	108.7
C32C—C31C—H31E	108.4	C32E—C31E—H31J	108.7
C30C—C31C—H31E	108.4	C30E—C31E—H31J	108.7
C32C—C31C—H31F	108.4	H31I—C31E—H31J	107.6
C30C—C31C—H31F	108.4	C31E—C32E—C33E	115 (3)
H31E—C31C—H31F	107.5	C31E—C32E—H32I	108.6
C31C—C32C—C33C	128 (3)	C33E—C32E—H32I	108.6
C31C—C32C—H32E	105.4	C31E—C32E—H32J	108.6
C33C—C32C—H32E	105.4	C33E—C32E—H32J	108.6
C31C—C32C—H32F	105.4	H32I—C32E—H32J	107.6
C33C—C32C—H32F	105.4	C34E—C33E—C32E	111 (3)
H32E—C32C—H32F	106.0	C34E—C33E—H33I	109.5
C34C—C33C—C32C	109 (3)	C32E—C33E—H33I	109.5
C34C—C33C—H33E	109.9	C34E—C33E—H33J	109.5
C32C—C33C—H33E	109.9	C32E—C33E—H33J	109.5
C34C—C33C—H33F	109.9	H33I—C33E—H33J	108.0
C32C—C33C—H33F	109.9	C33E—C34E—H34M	109.5
H33E—C33C—H33F	108.3	C33E—C34E—H34N	109.5

C33C—C34C—H34D	109.5	H34M—C34E—H34N	109.5
C33C—C34C—H34E	109.5	C33E—C34E—H34O	109.5
H34D—C34C—H34E	109.5	H34M—C34E—H34O	109.5
C33C—C34C—H34F	109.5	H34N—C34E—H34O	109.5
C2A—N1A—C1A—N2A	-5.7 (12)	C23A—N4A—C30A—C31A	102.0 (12)
C2C—N1A—C1A—N2A	4.0 (10)	C29A—N4A—C30A—C31A	-70.7 (14)
Hg1—N1A—C1A—N2A	176.1 (6)	N4A—C30A—C31A—C32A	-61.3 (16)
C2A—N1A—C1A—C13A	172.5 (11)	C30A—C31A—C32A—C33A	-172.0 (14)
C2C—N1A—C1A—C13A	-177.8 (9)	C31A—C32A—C33A—C34A	173.1 (16)
Hg1—N1A—C1A—C13A	-5.8 (12)	C23A—N4A—C30C—C31C	102.0 (12)
C7A—N2A—C1A—N1A	6 (2)	C29A—N4A—C30C—C31C	-70.7 (14)
C7C—N2A—C1A—N1A	-3.1 (13)	N4A—C30C—C31C—C32C	-61.3 (16)
C8A—N2A—C1A—N1A	-170.6 (9)	C30C—C31C—C32C—C33C	-176 (3)
C7A—N2A—C1A—C13A	-173 (2)	C31C—C32C—C33C—C34C	61 (8)
C7C—N2A—C1A—C13A	178.7 (11)	C23A—N4A—C30F—C31F	71 (2)
C8A—N2A—C1A—C13A	11.2 (15)	C29A—N4A—C30F—C31F	-102 (2)
C1A—N1A—C2A—C7A	3 (2)	N4A—C30F—C31F—C32F	48 (5)
Hg1—N1A—C2A—C7A	-178 (2)	C30F—C31F—C32F—C33F	68 (7)
C1A—N1A—C2A—C3A	-176 (2)	C31F—C32F—C33F—C34F	-172 (6)
Hg1—N1A—C2A—C3A	2 (2)	C2B—N1B—C1B—N2B	0.0 (10)
C7A—C2A—C3A—C4A	0 (4)	Hg1—N1B—C1B—N2B	-157.5 (6)
N1A—C2A—C3A—C4A	180 (2)	C2B—N1B—C1B—C13B	-179.8 (8)
C2A—C3A—C4A—C5A	1 (5)	Hg1—N1B—C1B—C13B	22.7 (12)
C3A—C4A—C5A—C6A	-2 (6)	C7B—N2B—C1B—N1B	0.5 (10)
C4A—C5A—C6A—C7A	2 (6)	C8B—N2B—C1B—N1B	-177.0 (9)
C1A—N2A—C7A—C2A	-3 (3)	C7B—N2B—C1B—C13B	-179.7 (8)
C8A—N2A—C7A—C2A	173.2 (15)	C8B—N2B—C1B—C13B	2.8 (14)
C1A—N2A—C7A—C6A	177 (4)	C1B—N1B—C2B—C3B	179.9 (11)
C8A—N2A—C7A—C6A	-7 (6)	Hg1—N1B—C2B—C3B	-22.6 (15)
N1A—C2A—C7A—N2A	0 (3)	C1B—N1B—C2B—C7B	-0.6 (10)
C3A—C2A—C7A—N2A	180 (2)	Hg1—N1B—C2B—C7B	157.0 (6)
N1A—C2A—C7A—C6A	180 (3)	N1B—C2B—C3B—C4B	178.0 (10)
C3A—C2A—C7A—C6A	0 (5)	C7B—C2B—C3B—C4B	-1.6 (16)
C5A—C6A—C7A—N2A	179 (4)	C2B—C3B—C4B—C5B	0.9 (17)
C5A—C6A—C7A—C2A	-1 (5)	C3B—C4B—C5B—C6B	-0.5 (17)
C1A—N1A—C2C—C7C	-3.5 (11)	C4B—C5B—C6B—C7B	0.9 (15)
Hg1—N1A—C2C—C7C	-175.1 (9)	C1B—N2B—C7B—C6B	177.4 (9)
C1A—N1A—C2C—C3C	174.8 (12)	C8B—N2B—C7B—C6B	-4.9 (15)
Hg1—N1A—C2C—C3C	3.3 (14)	C1B—N2B—C7B—C2B	-0.8 (10)
C7C—C2C—C3C—C4C	-1 (2)	C8B—N2B—C7B—C2B	176.8 (8)
N1A—C2C—C3C—C4C	-179.3 (12)	C5B—C6B—C7B—N2B	-179.6 (9)
C2C—C3C—C4C—C5C	0 (3)	C5B—C6B—C7B—C2B	-1.6 (14)
C3C—C4C—C5C—C6C	3 (3)	C3B—C2B—C7B—N2B	-179.5 (9)
C4C—C5C—C6C—C7C	-4 (3)	N1B—C2B—C7B—N2B	0.9 (10)
C1A—N2A—C7C—C2C	0.7 (15)	C3B—C2B—C7B—C6B	2.0 (15)
C8A—N2A—C7C—C2C	169.0 (10)	N1B—C2B—C7B—C6B	-177.6 (8)
C1A—N2A—C7C—C6C	-175.3 (18)	C1B—N2B—C8B—C9B	113.5 (10)

C8A—N2A—C7C—C6C	-7 (3)	C7B—N2B—C8B—C9B	-63.7 (13)
C3C—C2C—C7C—N2A	-176.9 (11)	N2B—C8B—C9B—C10B	162.5 (9)
N1A—C2C—C7C—N2A	1.7 (14)	C8B—C9B—C10B—C11B	-174.7 (10)
C3C—C2C—C7C—C6C	0 (2)	C9B—C10B—C11B—C12B	-179.5 (11)
N1A—C2C—C7C—C6C	178.1 (14)	N1B—C1B—C13B—C14B	49.8 (12)
C5C—C6C—C7C—N2A	178.3 (17)	N2B—C1B—C13B—C14B	-129.9 (9)
C5C—C6C—C7C—C2C	3 (3)	N1B—C1B—C13B—C18B	-127.5 (9)
C1A—N2A—C8A—C9A	-115.5 (11)	N2B—C1B—C13B—C18B	52.7 (12)
C7A—N2A—C8A—C9A	69 (3)	C18B—C13B—C14B—C15B	0.2 (12)
C7C—N2A—C8A—C9A	78.6 (15)	C1B—C13B—C14B—C15B	-177.2 (7)
N2A—C8A—C9A—C10A	-166.8 (10)	C13B—C14B—C15B—C16B	-2.0 (11)
C8A—C9A—C10A—C11A	76.3 (19)	C13B—C14B—C15B—C19B	-178.9 (7)
C9A—C10A—C11A—C12A	67.4 (19)	C14B—C15B—C16B—C17B	2.8 (11)
N1A—C1A—C13A—C18A	-119.2 (10)	C19B—C15B—C16B—C17B	179.7 (7)
N2A—C1A—C13A—C18A	58.7 (12)	C15B—C16B—C17B—C18B	-1.8 (12)
N1A—C1A—C13A—C14A	62.0 (12)	C15B—C16B—C17B—C23B	-178.3 (7)
N2A—C1A—C13A—C14A	-120.1 (10)	C16B—C17B—C18B—C13B	0.0 (11)
C18A—C13A—C14A—C15A	-1.2 (12)	C23B—C17B—C18B—C13B	176.3 (7)
C1A—C13A—C14A—C15A	177.6 (8)	C14B—C13B—C18B—C17B	0.8 (11)
C13A—C14A—C15A—C16A	1.0 (13)	C1B—C13B—C18B—C17B	178.1 (7)
C13A—C14A—C15A—C19A	-179.8 (8)	C16B—C15B—C19B—C20B	-99.9 (10)
C14A—C15A—C16A—C17A	0.6 (13)	C14B—C15B—C19B—C20B	77.0 (10)
C19A—C15A—C16A—C17A	-178.6 (8)	C16B—C15B—C19B—C22B	20.3 (11)
C15A—C16A—C17A—C18A	-2.2 (13)	C14B—C15B—C19B—C22B	-162.9 (8)
C15A—C16A—C17A—C23A	179.8 (8)	C16B—C15B—C19B—C21B	140.2 (8)
C14A—C13A—C18A—C17A	-0.3 (12)	C14B—C15B—C19B—C21B	-43.0 (11)
C1A—C13A—C18A—C17A	-179.1 (7)	C24B—N3B—C23B—N4B	0.4 (10)
C16A—C17A—C18A—C13A	2.0 (12)	Hg ₂ —N3B—C23B—N4B	-171.3 (5)
C23A—C17A—C18A—C13A	180.0 (8)	C24B—N3B—C23B—C17B	-179.3 (8)
C16A—C15A—C19A—C20C	-139.5 (19)	Hg ₂ —N3B—C23B—C17B	9.0 (11)
C14A—C15A—C19A—C20C	41 (2)	C29B—N4B—C23B—N3B	-0.9 (10)
C16A—C15A—C19A—C22A	61.1 (17)	C30B—N4B—C23B—N3B	169.3 (12)
C14A—C15A—C19A—C22A	-118.1 (16)	C30E—N4B—C23B—N3B	-167 (3)
C16A—C15A—C19A—C21C	-9 (2)	C30D—N4B—C23B—N3B	-154 (2)
C14A—C15A—C19A—C21C	171.7 (17)	C29B—N4B—C23B—C17B	178.8 (8)
C16A—C15A—C19A—C20A	-176.0 (15)	C30B—N4B—C23B—C17B	-11.0 (17)
C14A—C15A—C19A—C20A	4.8 (18)	C30E—N4B—C23B—C17B	12 (3)
C16A—C15A—C19A—C21A	-57.8 (15)	C30D—N4B—C23B—C17B	26 (2)
C14A—C15A—C19A—C21A	123.1 (13)	C18B—C17B—C23B—N3B	-118.7 (9)
C16A—C15A—C19A—C22C	101.9 (15)	C16B—C17B—C23B—N3B	57.6 (11)
C14A—C15A—C19A—C22C	-77.3 (15)	C18B—C17B—C23B—N4B	61.6 (11)
C24A—N3A—C23A—N4A	0.8 (10)	C16B—C17B—C23B—N4B	-122.0 (9)
Hg ₂ ⁱⁱ —N3A—C23A—N4A	-163.3 (6)	C23B—N3B—C24B—C29B	0.3 (10)
C24A—N3A—C23A—C17A	-175.7 (8)	Hg ₂ —N3B—C24B—C29B	171.3 (6)
Hg ₂ ⁱⁱ —N3A—C23A—C17A	20.2 (12)	C23B—N3B—C24B—C25B	178.7 (12)
C29A—N4A—C23A—N3A	-0.8 (11)	Hg ₂ —N3B—C24B—C25B	-10.3 (16)
C30F—N4A—C23A—N3A	-174.5 (9)	C29B—C24B—C25B—C26B	-2.6 (19)
C30A—N4A—C23A—N3A	-174.5 (9)	N3B—C24B—C25B—C26B	179.2 (12)

C30C—N4A—C23A—N3A	-174.5 (9)	C24B—C25B—C26B—C27B	4 (2)
C29A—N4A—C23A—C17A	175.6 (9)	C25B—C26B—C27B—C28B	-3 (2)
C30F—N4A—C23A—C17A	1.9 (15)	C26B—C27B—C28B—C29B	0.9 (18)
C30A—N4A—C23A—C17A	1.9 (15)	C23B—N4B—C29B—C24B	1.1 (10)
C30C—N4A—C23A—C17A	1.9 (15)	C30B—N4B—C29B—C24B	-170.7 (11)
C16A—C17A—C23A—N3A	57.1 (12)	C30E—N4B—C29B—C24B	165 (3)
C18A—C17A—C23A—N3A	-120.9 (9)	C30D—N4B—C29B—C24B	154 (2)
C16A—C17A—C23A—N4A	-118.9 (10)	C23B—N4B—C29B—C28B	-178.6 (10)
C18A—C17A—C23A—N4A	63.1 (12)	C30B—N4B—C29B—C28B	9.6 (17)
C23A—N3A—C24A—C29A	-0.5 (10)	C30E—N4B—C29B—C28B	-15 (4)
Hg2 ⁱⁱ —N3A—C24A—C29A	163.7 (6)	C30D—N4B—C29B—C28B	-26 (2)
C23A—N3A—C24A—C25A	179.1 (9)	N3B—C24B—C29B—N4B	-0.9 (10)
Hg2 ⁱⁱ —N3A—C24A—C25A	-16.7 (13)	C25B—C24B—C29B—N4B	-179.4 (10)
C29A—C24A—C25A—C26A	-1.2 (13)	N3B—C24B—C29B—C28B	178.9 (9)
N3A—C24A—C25A—C26A	179.2 (9)	C25B—C24B—C29B—C28B	0.3 (15)
C24A—C25A—C26A—C27A	-0.6 (14)	C27B—C28B—C29B—N4B	-179.8 (11)
C25A—C26A—C27A—C28A	1.7 (16)	C27B—C28B—C29B—C24B	0.5 (16)
C26A—C27A—C28A—C29A	-0.8 (16)	C23B—N4B—C30B—C31B	-102.4 (15)
C23A—N4A—C29A—C24A	0.4 (11)	C29B—N4B—C30B—C31B	67.0 (15)
C30F—N4A—C29A—C24A	174.4 (9)	N4B—C30B—C31B—C32B	-172.4 (13)
C30A—N4A—C29A—C24A	174.4 (9)	C30B—C31B—C32B—C33B	-178.2 (16)
C30C—N4A—C29A—C24A	174.4 (9)	C31B—C32B—C33B—C34B	177.1 (17)
C23A—N4A—C29A—C28A	178.5 (11)	C23B—N4B—C30D—C31D	-154 (2)
C30F—N4A—C29A—C28A	-7.6 (18)	C29B—N4B—C30D—C31D	57 (4)
C30A—N4A—C29A—C28A	-7.6 (18)	N4B—C30D—C31D—C32D	106 (5)
C30C—N4A—C29A—C28A	-7.6 (18)	C30D—C31D—C32D—C33D	-153 (5)
N3A—C24A—C29A—N4A	0.0 (11)	C31D—C32D—C33D—C34D	120 (5)
C25A—C24A—C29A—N4A	-179.6 (8)	C23B—N4B—C30E—C31E	94 (5)
N3A—C24A—C29A—C28A	-178.2 (9)	C29B—N4B—C30E—C31E	-68 (7)
C25A—C24A—C29A—C28A	2.1 (15)	N4B—C30E—C31E—C32E	165 (5)
C27A—C28A—C29A—N4A	-178.9 (10)	C30E—C31E—C32E—C33E	168 (6)
C27A—C28A—C29A—C24A	-1.1 (16)	C31E—C32E—C33E—C34E	-179 (6)

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3A—H3AA \cdots N1B	0.95	2.45	3.29 (4)	148
C8A—H8AB \cdots Br22 ⁱⁱ	0.99	2.94	3.873 (11)	158
C25A—H25A \cdots Br21 ⁱⁱ	0.95	2.96	3.66 (2)	131
C25A—H25A \cdots Cl21 ⁱⁱ	0.95	2.74	3.45 (3)	132
C28A—H28A \cdots Br11 ⁱⁱⁱ	0.95	2.96	3.793 (12)	147
C28A—H28A \cdots Cl11 ⁱⁱⁱ	0.95	2.86	3.70 (2)	149
C30A—H30B \cdots Br11 ⁱⁱⁱ	0.99	3.04	3.979 (13)	158
C3B—H3BA \cdots Br11	0.95	2.96	3.631 (11)	129
C6B—H6BA \cdots Br21 ^{iv}	0.95	2.88	3.75 (2)	153
C6B—H6BA \cdots Cl21 ^{iv}	0.95	2.89	3.73 (4)	149

<i>C25B</i> — <i>H25B</i> ··· <i>N3A</i> ⁱ	0.95	2.56	3.332 (14)	139
<i>C30D</i> — <i>H30G</i> ··· <i>Br12</i>	0.99	3.06	3.95 (5)	150

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$; (iii) $x-1/2, -y+1, z$; (iv) $x+1/2, -y, z$.