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1,4-Diiodoperchlorobenzene behaves as a dual π-type halogen-bond donor to stilbene in the organic solid state

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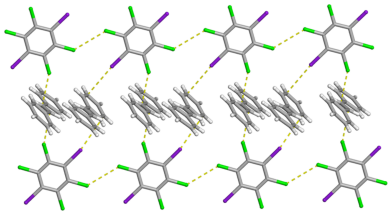
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The synthesis and crystal structure of a halogen-bonded co-crystal based upon 1,4-diiodoperchlorobenzene ($C_6I_2Cl_4$) and stilbene (stil) are described. The resulting co-crystal {systematic name: 1,4-diiodo-2,3,5,6-tetrachlorobenzene–1,1′-[(*E*)-ethene-1,2-diyl]dibenzene (2/1)}, $2C_6I_2Cl_4$·stil is held together primarily by two varieties of π-type halogen bonds between the molecular components. Each aromatic ring within stil accepts two C—I$\cdots\pi$ halogen bonds on opposite sides to form a two-dimensional offset bordered stacked pattern. In addition, the donor $C_6I_2Cl_4$ also engages in a C—Cl$\cdots\pi$ halogen bond to the ethylene group. Lastly, neighbouring molecules of $C_6I_2Cl_4$ interact by means of Type I chlorine–chlorine contacts, which results in a three-dimensional extended structure.

1. Chemical context

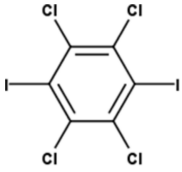
Co-crystals remain an important class of organic solids where at least two molecular components are found in a fixed and whole number ratio within the crystal structure (Corpinot & Bučar, 2019). The formation of these multi-component molecular solids relies on supramolecular interactions between complementary donor and acceptor sites as a driving force to the self-assembly process. In particular, halogen bonding has proven to be a reliable non-covalent interaction to facilitate co-crystal formation (Gilday *et al.*, 2015). Halogen bonds are defined as an attractive interaction between an electrophilic region at the tip of the halogen atom bond to a carbon atom (*i.e.* the σ-hole) and a nucleophilic region usually on a second molecule (Cavallo *et al.*, 2016). Analysis of previously reported crystal structures revealed that the most common variety of halogen bonds is classified as *n*-type involving a polarizable halogen atom and a lone pair of electrons on oxygen or nitrogen (Walsh *et al.*, 2001). Despite the prevalence of *n*-type interactions, a less reported class of halogen bonding interactions is called π-type involving a halogen atom and an electron-rich surface such as a polycyclic aromatic (Vainauskas & Friščić, 2026; Vainauskas *et al.*, 2020, 2023; d'Agostino *et al.*, 2015; Shen *et al.*, 2012).

A continued focus between our research groups has been the intentional design of co-crystals that utilize π-type halogen bonds as the primary non-covalent interaction in the formation of multi-component molecular solids. To this end, we have reported on the ability of 1,4-diiodoperchlorobenzene ($C_6I_2Cl_4$) to behave as a π-type halogen-bond donor to various aromatics including benzene (Bosch, 2019), naphthalene (Bosch *et al.*, 2023), benzamide (Feld *et al.*, 2026), as well as

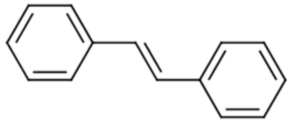


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benzoic and cinnamic acids (Feld *et al.*, 2025) to generate co-crystals. With the goal to expand this research to other related aromatic systems, herein, we report the synthesis, crystal structure, and Hirshfeld surface analysis of a co-crystal based upon $C_6I_2Cl_4$ along with stilbene (stil). In particular, the co-crystal $2C_6I_2Cl_4$·stil is sustained by the combination of C—I···π and C—Cl···π halogen bonds along with Type I chlorine–chlorine contacts that results in a three-dimensional extended molecular solid.



$C_6I_2Cl_4$



stil

2. Structural commentary

Crystallographic analysis reveals that $2C_6I_2Cl_4$·stil crystallizes in the centrosymmetric triclinic space group $P\overline{1}$. The asymmetric unit contains two molecules of $C_6I_2Cl_4$ and one of stil (Fig. 1). The co-crystal is sustained by four unique C—I···π halogen bonds with distances of 3.393 (1), 3.401 (1), 3.540 (1), and 3.569 (1) Å between an I atom and an aromatic ring. These halogen-bond distances were determined by using the I atom on $C_6I_2Cl_4$ and the calculated plane for the nearest aromatic ring on stil. Further support of the formation of these C—I···π halogen bonds are the nearly perpendicular angles for this non-covalent interaction with values of 84.96 (7), 86.25 (6), 96.39 (6), and 106.38 (6)° (Fig. 2). As expected, both crystallographically unique $C_6I_2Cl_4$ molecules form two C—I···π halogen bonds with two different stil molecules, generating a two-dimensional sheet-like structure that can be classified as an offset bordered stack pattern (Fig. 2). In addition, these molecular components also engage in C—Cl···π halogen bonds between $C_6I_2Cl_4$ and the ethylene group within stil at a distance of 3.264 (7) Å. This value was determined by using a Cl atom and the centroid of the ethylene group. The stil molecule is found to be positionally disordered over two locations, which is common for similarly shaped molecules (Harada & Ogawa, 2014). A free-variable refinement determined the occupancies for this observed disorder and returned values of 0.55 and 0.45 at 100 K. These bond distances for each π-type halogen bonds were determined by using the major configuration for the disordered benzene rings.

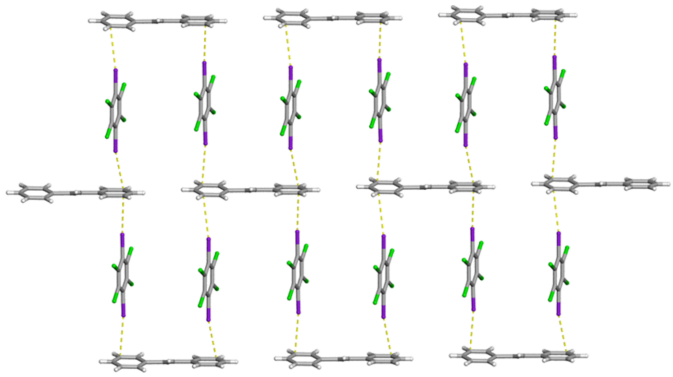


Figure 2
X-ray crystal structure $2C_6I_2Cl_4$·stil illustrating the offset bordered stack pattern along with C—I···π halogen bonds. The crystallographic disorder within stil was omitted for clarity.

3. Supramolecular features

In addition to the two different π-type halogen bonds, the halogen-bond donor $C_6I_2Cl_4$ is also found to engage in Type I chlorine–chlorine contacts within $2C_6I_2Cl_4$·stil (Fig. 3). Each donor is engaged in two unique Type I chlorine–chlorine contacts found between Cl6···Cl8 at a distance of 3.460 (1) Å with C—Cl···Cl bond angles of 132.05 (10) and 132.13 (11)° [symmetry code: Cl8 ($x-1, y, z$)] as well as between Cl2···Cl4 with a bond length of 3.488 (1) Å with angles of 131.11 (13) and 131.33 (11)° [symmetry code: Cl4 ($1+x, y, z$)] (Mukherjee *et al.*, 2014). By definition, a Type I halogen–halogen contact will have nearly identical C—X···X bond angles while a Type

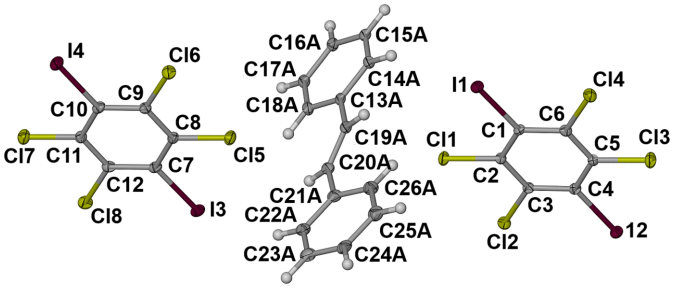


Figure 1
The labelled asymmetric unit of $2C_6I_2Cl_4$·stil. Displacement ellipsoids are drawn at the 50% probability level for non-hydrogen atoms while hydrogen atoms are shown as spheres of arbitrary size. The crystallographic disorder within stil was omitted for clarity.

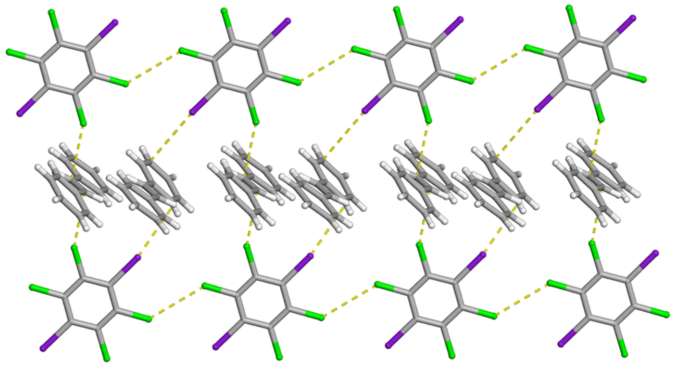


Figure 3
X-ray crystal structure of $2C_6I_2Cl_4$·stil illustrating Type I chlorine–chlorine contacts along with both C—I···π and C—Cl···π halogen bonds. The crystallographic disorder within stil was omitted for clarity.

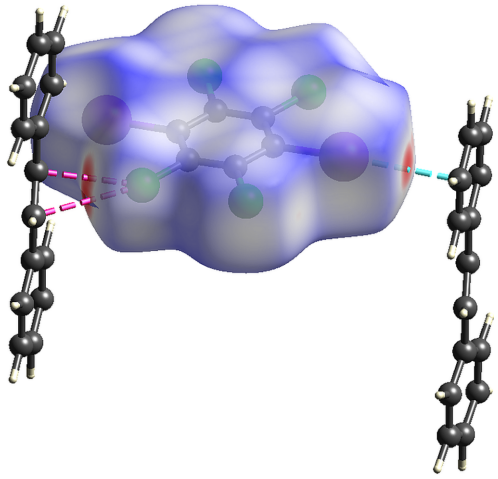


Figure 4
Hirshfeld surface of $2C_6I_2Cl_4$·stil where d_{norm} is mapped onto the surface illustrating the C—I···π halogen bonds (light blue dashes) and C—Cl···π halogen bonds (light pink dashes). The crystallographic disorder within stil was omitted for clarity.

II halogen–halogen contact will have C—X···X bond angles near 90 and 180° (Scheiner, 2022).

The different π-type halogen bonds were also investigated and visualized by utilizing a Hirshfeld surface analysis (Spackman *et al.*, 2021) where d_{norm} is mapped onto the calculated surface (Fig. 4). The red spots on the Hirshfeld surface represent both examples for these π-type halogen bonds. This Hirshfeld surface analysis along with the observed bond lengths confirms the presence of both C—I···π and C—Cl···π halogen bonds within $2C_6I_2Cl_4$·stil.

4. Database survey

A search of the Cambridge Structural Database (CSD Version 2026.2.0 Build 506344; Groom *et al.*, 2016) using Conquest (Bruno *et al.*, 2002) for structures containing 1,4-diiodoperchlorobenzene ($C_6I_2Cl_4$) in which the I atom is within the van der Waals radius of an aromatic surface revealed only five structures that are classified as a co-crystal. These π-type halogen-bonded co-crystals contained benzene (refcode HONBIY; Bosch, 2019), naphthalene (GOCCUA; Bosch *et al.*, 2023), benzoic acid (PAHQID; Feld *et al.*, 2025), cinnamic acid (PAHQOJ; Feld *et al.*, 2025), and benzamide (WADJOF; Feld *et al.*, 2026). In all of these co-crystals, the solid is primarily held together by C—I···π halogen bonds. A similar crystal structure was reported based upon 1,4-diiodoperfluorobenzene and stil, which resulted in a related, but not isostructural, two-dimensional offset bordered stacked pattern (GUFNUS; d'Agostino *et al.*, 2015).

5. Synthesis and crystallization

Materials and general methods

Toluene and the halogen-bond acceptor stilbene (stil) were purchased from Sigma-Aldrich Chemical (St. Louis, MO, USA) and used as received. The halogen-bond donor 1,4-diiodoperchlorobenzene ($C_6I_2Cl_4$) was synthesized utilizing a previously published method (Reddy *et al.*, 2006).

Synthesis and crystallization

The formation of $2C_6I_2Cl_4$·stil was achieved by dissolving 50.0 mg of $C_6I_2Cl_4$ in 2.0 mL of toluene and then combining the resulting solution with 9.6 mg of stil (2:1 molar ratio) under ambient conditions. Within two days, single crystals suitable for X-ray diffraction were formed upon loss of solvent by slow evaporation at room temperature.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{12}·2C_6Cl_4I_2$
M_r	1115.56
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	8.9485 (7), 13.459 (1), 14.3024 (10)
α, β, γ (°)	63.799 (2), 83.697 (3), 89.960 (3)
V (Å^3)	1534.0 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.78
Crystal size (mm)	0.20 × 0.18 × 0.13
Data collection	
Diffractometer	Bruker D8 Venture Duo with Photon III
Absorption correction	Numerical (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.477, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	81922, 9290, 7508
R_{int}	0.067
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.714
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.066, 1.08
No. of reflections	9290
No. of parameters	423
No. of restraints	198
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.08, −1.05

Computer programs: *APEX5* and *SAINT* (Bruker, 2024), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2025/1* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 1. The stilbene molecule (C13–C26) was positionally disordered and modeled as split sites *A* and *B*. The occupancies for the *A* and *B* sites refined to 0.545 (9) and 0.455 (9), respectively. To help maintain reasonable ADP and bond length values for the disordered atom sites, the rigid-bond restraint RIGU and C—C bond-length constraint AFIX 66 were applied. Hydrogen atoms were located in difference-Fourier maps and were geometrically constrained using the appropriate AFIX commands.

Acknowledgements

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References

Bosch, E. (2019). *IUCrData* **4**, x190993.

Bosch, E., Reinheimer, E. W., Unruh, D. K. & Groeneman, R. H. (2023). *Acta Cryst.* E**79**, 958–961.

Bruker (2024). *APEX5* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.

Cavallo, G., Metrangolo, P., Milani, R., Pilati, T., Priimagi, A., Resnati, G. & Terraneo, G. (2016). *Chem. Rev.* **116**, 2478–2601.

Corpinot, M. K. & Bučar, D.-K. (2019). *Cryst. Growth Des.* **19**, 1426–1453.

d'Agostino, S., Grepioni, F., Braga, D. & Ventura, B. (2015). *Cryst. Growth Des.* **15**, 2039–2045.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Feld, E. H., Bosch, E., Unruh, D. K., Krueger, H. R. & Groeneman, R. H. (2025). *CrystEngComm* **27**, 5100–5103.

Feld, E. H., Bosch, E., Unruh, D. K., Krueger, H. R. & Groeneman, R. H. (2026). *CrystEngComm* **28**, 1770–1774.

Gilday, L. C., Robinson, S. W., Barendt, T. A., Langton, M. J., Mullaney, B. R. & Beer, P. D. (2015). *Chem. Rev.* **115**, 7118–7195.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Harada, J. & Ogawa, K. (2014). *Cryst. Growth Des.* **14**, 5182–5188.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.

Mukherjee, A., Tothadi, S. & Desiraju, G. R. (2014). *Acc. Chem. Res.* **47**, 2514–2524.

Reddy, C. M., Kirchner, M. T., Gundakaram, R. C., Padmanabhan, K. A. & Desiraju, G. R. (2006). *Chem. Eur. J.* **12**, 2222–2234.

Scheiner, S. (2022). *Cryst. Growth Des.* **22**, 2692–2702.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Shen, Q. J., Pang, X., Zhao, X. R., Gao, H. Y., Sun, H.-L. & Jin, W. J. (2012). *CrystEngComm* **14**, 5027–5034.

Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.

Vainauskas, J., Borchers, T. H., Arhangelskis, M., McCormick McPherson, L. J., Spilfogel, T. S., Hamzehpoor, E., Topić, F., Coles, S. J., Perepichka, D. F., Barrett, C. J. & Friščić, T. (2023). *Chem. Sci.* **14**, 13031–13041.

Vainauskas, J. & Friščić, T. (2026). *Chem. Commun.* **62**, 5780–5803.

Vainauskas, J., Topić, F., Bushuyev, O. S., Barrett, C. J. & Friščić, T. (2020). *Chem. Commun.* **56**, 15145–15148.

Walsh, R. B., Padgett, C. W., Metrangolo, P., Resnati, G., Hanks, T. W. & Pennington, W. T. (2001). *Cryst. Growth Des.* **1**, 165–175.

supporting information

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1,4-Diiodoperchlorobenzene behaves as a dual π-type halogen-bond donor to stilbene in the organic solid state

Eric Bosch, Eric W. Reinheimer, Daniel K. Unruh and Ryan H. Groeneman

Computing details

1,4-Diiodo-2,3,5,6-tetrachlorobenzene–1,1′-[(*E*)-ethene-1,2-diyl]dibenzene (2/1)

Crystal data

$C_{14}H_{12}·2C_6Cl_4I_2$
M_r = 1115.56
Triclinic, $P\overline{1}$
a = 8.9485 (7) Å
b = 13.459 (1) Å
c = 14.3024 (10) Å
α = 63.799 (2)°
β = 83.697 (3)°
γ = 89.960 (3)°
V = 1534.0 (2) Å^3
Z = 2
$F(000)$ = 1032
D_x = 2.415 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9838 reflections
θ = 2.8–30.5°
μ = 4.78 mm^{-1}
T = 100 K
Irregular, clear colourless
0.20 × 0.18 × 0.13 mm

Data collection

Bruker D8 Venture Duo with Photon III diffractometer
ω and φ scans
Absorption correction: numerical (SADABS; Krause *et al.*, 2015)
T_{min} = 0.477, T_{max} = 0.746
81922 measured reflections
9290 independent reflections
7508 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 30.5°, θ_{min} = 2.3°
h = −12→12
k = −19→19
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.066
S = 1.08
9290 reflections
423 parameters
198 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 3.9009P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −1.05 e Å^{-3}
Extinction correction: SHELXL2025/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0036 (2)

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. Intensity data were corrected for Lorentz, polarization, and background effects using the APEX5 (Bruker, 2023). A numerical absorption correction was applied based on a Gaussian integration over a multifaceted crystal and followed by a semi-empirical correction for adsorption applied using SADABS (Bruker, 2023). The program SHELXT (Sheldrick, 2015a) was used for the initial structure solution and SHELXL (Sheldrick, 2015b) was used for the refinement of the structure. Both programs were utilized within the OLEX2 software (Dolomanov *et al.*, 2009).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
I1	−0.04912 (2)	0.20487 (2)	0.47628 (2)	0.01794 (5)	
I2	0.55655 (2)	0.02741 (2)	0.24486 (2)	0.01832 (5)	
Cl1	0.31062 (8)	0.21810 (7)	0.51139 (6)	0.01932 (15)	
Cl2	0.57843 (8)	0.14273 (7)	0.40908 (6)	0.01868 (14)	
Cl3	0.19653 (9)	0.01174 (7)	0.21137 (6)	0.02307 (16)	
Cl4	−0.07171 (8)	0.08774 (7)	0.31359 (6)	0.02010 (15)	
C1	0.1313 (3)	0.1496 (3)	0.4082 (2)	0.0146 (5)	
C2	0.2780 (3)	0.1605 (2)	0.4294 (2)	0.0138 (5)	
C3	0.3997 (3)	0.1262 (2)	0.3822 (2)	0.0138 (5)	
C4	0.3760 (3)	0.0801 (2)	0.3143 (2)	0.0150 (5)	
C5	0.2297 (3)	0.0692 (3)	0.2940 (2)	0.0153 (6)	
C6	0.1073 (3)	0.1035 (3)	0.3406 (2)	0.0154 (5)	
I3	0.56573 (2)	0.55378 (2)	0.77449 (2)	0.01940 (6)	
I4	−0.03827 (2)	0.72402 (2)	1.01342 (2)	0.02170 (6)	
Cl5	0.20522 (9)	0.53666 (7)	0.74433 (6)	0.02139 (15)	
Cl6	−0.06169 (8)	0.60976 (7)	0.84944 (6)	0.02174 (15)	
Cl7	0.32291 (9)	0.74258 (7)	1.04409 (6)	0.02217 (15)	
Cl8	0.59085 (8)	0.67057 (7)	0.93758 (6)	0.02108 (15)	
C7	0.3863 (3)	0.6059 (3)	0.8459 (2)	0.0165 (6)	
C8	0.2392 (3)	0.5933 (3)	0.8271 (2)	0.0156 (5)	
C9	0.1182 (3)	0.6269 (3)	0.8748 (2)	0.0159 (6)	
C10	0.1424 (3)	0.6738 (3)	0.9420 (2)	0.0167 (6)	
C11	0.2894 (3)	0.6857 (3)	0.9612 (2)	0.0162 (6)	
C12	0.4110 (3)	0.6525 (3)	0.9132 (2)	0.0165 (6)	
C13A	0.2242 (8)	0.2358 (5)	0.7545 (5)	0.0164 (13)	0.545 (9)
C18A	0.3236 (9)	0.2389 (5)	0.8215 (6)	0.0191 (14)	0.545 (9)
H18A	0.384475	0.304224	0.802594	0.023*	0.545 (9)
C17A	0.3338 (12)	0.1462 (7)	0.9161 (6)	0.0205 (18)	0.545 (9)
H17A	0.401751	0.148287	0.961933	0.025*	0.545 (9)
C16A	0.2447 (14)	0.0506 (7)	0.9438 (7)	0.021 (2)	0.545 (9)
H16A	0.251736	−0.012732	1.008487	0.025*	0.545 (9)
C15A	0.1453 (12)	0.0476 (6)	0.8768 (7)	0.0198 (16)	0.545 (9)
H15A	0.084444	−0.017815	0.895704	0.024*	0.545 (9)
C14A	0.1351 (9)	0.1402 (6)	0.7822 (6)	0.0191 (14)	0.545 (9)

H14A	0.067165	0.138121	0.736365	0.023*	0.545 (9)
C19A	0.2082 (7)	0.3332 (5)	0.6522 (5)	0.0185 (12)	0.545 (9)
H19A	0.123192	0.329812	0.619117	0.022*	0.545 (9)
C20A	0.3000 (6)	0.4254 (5)	0.6012 (5)	0.0195 (13)	0.545 (9)
H20A	0.384581	0.430205	0.634061	0.023*	0.545 (9)
C21A	0.2815 (7)	0.5209 (4)	0.4979 (4)	0.0208 (13)	0.545 (9)
C26A	0.1931 (8)	0.5089 (4)	0.4291 (5)	0.0235 (14)	0.545 (9)
H26A	0.144999	0.438933	0.446753	0.028*	0.545 (9)
C25A	0.1752 (9)	0.5992 (6)	0.3344 (5)	0.0260 (17)	0.545 (9)
H25A	0.114810	0.591022	0.287317	0.031*	0.545 (9)
C24A	0.2456 (12)	0.7016 (5)	0.3085 (5)	0.0252 (18)	0.545 (9)
H24A	0.233377	0.763354	0.243741	0.030*	0.545 (9)
C23A	0.3340 (10)	0.7136 (5)	0.3773 (6)	0.0273 (18)	0.545 (9)
H23A	0.382134	0.783597	0.359600	0.033*	0.545 (9)
C22A	0.3519 (8)	0.6233 (6)	0.4720 (5)	0.0234 (14)	0.545 (9)
H22A	0.412325	0.631509	0.519036	0.028*	0.545 (9)
C13B	0.2661 (10)	0.2484 (6)	0.7610 (6)	0.0162 (16)	0.455 (9)
C18B	0.3513 (12)	0.2286 (7)	0.8425 (7)	0.0212 (18)	0.455 (9)
H18B	0.422665	0.283894	0.836732	0.025*	0.455 (9)
C17B	0.3322 (16)	0.1280 (9)	0.9324 (8)	0.023 (2)	0.455 (9)
H17B	0.390444	0.114475	0.988145	0.027*	0.455 (9)
C16B	0.2278 (17)	0.0471 (8)	0.9409 (8)	0.022 (3)	0.455 (9)
H16B	0.214753	−0.021672	1.002361	0.026*	0.455 (9)
C15B	0.1426 (14)	0.0669 (7)	0.8594 (9)	0.021 (2)	0.455 (9)
H15B	0.071282	0.011600	0.865165	0.026*	0.455 (9)
C14B	0.1617 (11)	0.1675 (7)	0.7695 (7)	0.0177 (17)	0.455 (9)
H14B	0.103502	0.181018	0.713752	0.021*	0.455 (9)
C19B	0.2907 (8)	0.3570 (6)	0.6645 (6)	0.0185 (15)	0.455 (9)
H19B	0.375813	0.402484	0.658540	0.022*	0.455 (9)
C20B	0.2055 (8)	0.3969 (6)	0.5854 (6)	0.0202 (15)	0.455 (9)
H20B	0.120806	0.351490	0.590572	0.024*	0.455 (9)
C21B	0.2312 (9)	0.5063 (5)	0.4899 (5)	0.0185 (15)	0.455 (9)
C26B	0.1556 (8)	0.5220 (6)	0.4050 (6)	0.0223 (16)	0.455 (9)
H26B	0.091480	0.463885	0.408493	0.027*	0.455 (9)
C25B	0.1737 (12)	0.6226 (7)	0.3150 (6)	0.025 (2)	0.455 (9)
H25B	0.122032	0.633257	0.256987	0.030*	0.455 (9)
C24B	0.2675 (14)	0.7075 (6)	0.3099 (7)	0.029 (3)	0.455 (9)
H24B	0.279923	0.776299	0.248434	0.035*	0.455 (9)
C23B	0.3432 (12)	0.6919 (6)	0.3949 (7)	0.025 (2)	0.455 (9)
H23B	0.407264	0.749971	0.391387	0.030*	0.455 (9)
C22B	0.3250 (9)	0.5913 (6)	0.4849 (5)	0.0200 (16)	0.455 (9)
H22B	0.376714	0.580600	0.542894	0.024*	0.455 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01274 (9)	0.02108 (11)	0.02154 (10)	0.00238 (7)	0.00084 (7)	−0.01153 (8)
I2	0.01449 (9)	0.02051 (11)	0.02214 (10)	0.00274 (7)	0.00125 (7)	−0.01222 (8)

Cl1	0.0171 (3)	0.0269 (4)	0.0206 (3)	0.0017 (3)	−0.0034 (3)	−0.0162 (3)
Cl2	0.0113 (3)	0.0247 (4)	0.0232 (3)	0.0009 (3)	−0.0034 (3)	−0.0132 (3)
Cl3	0.0200 (4)	0.0316 (4)	0.0275 (4)	0.0025 (3)	−0.0050 (3)	−0.0216 (4)
Cl4	0.0121 (3)	0.0266 (4)	0.0261 (4)	0.0011 (3)	−0.0049 (3)	−0.0151 (3)
C1	0.0123 (13)	0.0169 (14)	0.0153 (13)	0.0006 (11)	0.0012 (10)	−0.0085 (12)
C2	0.0124 (13)	0.0153 (14)	0.0147 (13)	0.0013 (10)	−0.0022 (10)	−0.0074 (11)
C3	0.0114 (13)	0.0146 (14)	0.0155 (13)	0.0018 (10)	−0.0020 (10)	−0.0067 (11)
C4	0.0142 (13)	0.0133 (14)	0.0167 (13)	0.0029 (10)	−0.0005 (10)	−0.0061 (11)
C5	0.0159 (14)	0.0158 (14)	0.0155 (13)	−0.0011 (11)	−0.0007 (10)	−0.0082 (12)
C6	0.0121 (13)	0.0173 (15)	0.0167 (13)	0.0007 (11)	−0.0031 (10)	−0.0072 (12)
I3	0.01607 (10)	0.01981 (11)	0.02102 (10)	0.00361 (7)	0.00331 (7)	−0.00915 (8)
I4	0.01700 (10)	0.02612 (12)	0.02600 (11)	0.00460 (8)	0.00189 (8)	−0.01622 (9)
Cl5	0.0212 (4)	0.0259 (4)	0.0223 (4)	0.0025 (3)	−0.0011 (3)	−0.0159 (3)
Cl6	0.0147 (3)	0.0272 (4)	0.0271 (4)	0.0026 (3)	−0.0018 (3)	−0.0157 (3)
Cl7	0.0218 (4)	0.0258 (4)	0.0244 (4)	0.0035 (3)	−0.0030 (3)	−0.0161 (3)
Cl8	0.0140 (3)	0.0253 (4)	0.0243 (4)	0.0020 (3)	−0.0023 (3)	−0.0114 (3)
C7	0.0156 (14)	0.0149 (14)	0.0165 (13)	0.0029 (11)	0.0010 (11)	−0.0054 (12)
C8	0.0169 (14)	0.0146 (14)	0.0155 (13)	0.0013 (11)	0.0003 (10)	−0.0074 (12)
C9	0.0120 (13)	0.0172 (15)	0.0194 (14)	0.0010 (11)	−0.0001 (10)	−0.0094 (12)
C10	0.0164 (14)	0.0159 (15)	0.0166 (13)	0.0041 (11)	0.0008 (11)	−0.0068 (12)
C11	0.0175 (14)	0.0151 (14)	0.0163 (13)	0.0014 (11)	−0.0011 (11)	−0.0074 (12)
C12	0.0132 (13)	0.0159 (15)	0.0173 (13)	0.0018 (11)	−0.0011 (10)	−0.0048 (12)
C13A	0.012 (4)	0.021 (2)	0.023 (2)	−0.0007 (17)	0.0002 (18)	−0.0162 (16)
C18A	0.017 (3)	0.021 (3)	0.026 (3)	−0.001 (2)	−0.003 (2)	−0.017 (2)
C17A	0.016 (4)	0.024 (3)	0.027 (3)	0.002 (2)	−0.001 (3)	−0.016 (2)
C16A	0.020 (4)	0.023 (3)	0.023 (3)	0.001 (3)	0.001 (3)	−0.014 (2)
C15A	0.015 (3)	0.024 (3)	0.023 (3)	−0.002 (2)	0.005 (2)	−0.014 (2)
C14A	0.016 (3)	0.023 (3)	0.023 (3)	−0.006 (2)	0.002 (2)	−0.016 (2)
C19A	0.015 (3)	0.022 (2)	0.023 (2)	0.0006 (17)	0.0006 (17)	−0.0144 (15)
C20A	0.015 (3)	0.022 (2)	0.024 (2)	0.0005 (17)	0.0016 (17)	−0.0139 (16)
C21A	0.015 (3)	0.023 (2)	0.024 (2)	−0.0002 (18)	0.0037 (18)	−0.0118 (16)
C26A	0.020 (3)	0.025 (3)	0.025 (3)	0.001 (2)	0.001 (2)	−0.012 (2)
C25A	0.029 (4)	0.024 (3)	0.026 (3)	0.006 (2)	−0.001 (3)	−0.013 (2)
C24A	0.027 (4)	0.023 (3)	0.025 (3)	0.005 (3)	0.006 (2)	−0.013 (2)
C23A	0.030 (4)	0.024 (3)	0.024 (3)	−0.005 (3)	0.009 (2)	−0.010 (2)
C22A	0.019 (3)	0.023 (3)	0.025 (3)	−0.004 (2)	0.008 (2)	−0.011 (2)
C13B	0.015 (4)	0.018 (2)	0.021 (2)	−0.003 (2)	0.001 (2)	−0.0139 (18)
C18B	0.016 (4)	0.028 (3)	0.024 (3)	−0.003 (3)	−0.003 (2)	−0.014 (2)
C17B	0.023 (5)	0.028 (4)	0.020 (3)	−0.002 (3)	0.000 (3)	−0.014 (2)
C16B	0.020 (5)	0.022 (4)	0.026 (4)	0.000 (3)	0.000 (3)	−0.014 (3)
C15B	0.020 (4)	0.020 (3)	0.027 (4)	−0.003 (3)	0.000 (3)	−0.013 (3)
C14B	0.014 (4)	0.018 (3)	0.026 (3)	−0.002 (2)	−0.001 (3)	−0.015 (2)
C19B	0.018 (3)	0.018 (2)	0.023 (2)	−0.002 (2)	0.0001 (19)	−0.0128 (17)
C20B	0.020 (3)	0.021 (3)	0.021 (2)	−0.002 (2)	−0.0002 (19)	−0.0114 (18)
C21B	0.014 (4)	0.020 (2)	0.022 (2)	0.002 (2)	0.004 (2)	−0.0102 (17)
C26B	0.019 (4)	0.023 (3)	0.023 (3)	0.003 (3)	0.000 (2)	−0.010 (2)
C25B	0.020 (4)	0.027 (4)	0.023 (3)	0.003 (3)	0.002 (3)	−0.006 (2)
C24B	0.027 (5)	0.025 (4)	0.025 (4)	0.000 (3)	−0.001 (3)	−0.003 (3)

C23B	0.018 (4)	0.025 (3)	0.021 (3)	−0.001 (3)	0.004 (3)	−0.003 (3)
C22B	0.017 (4)	0.020 (3)	0.019 (3)	−0.001 (2)	0.005 (2)	−0.007 (2)

Geometric parameters (Å, º)

I1—C1	2.097 (3)	C20A—C21A	1.497 (7)
I2—C4	2.089 (3)	C21A—C26A	1.3900
Cl1—C2	1.715 (3)	C21A—C22A	1.3900
Cl2—C3	1.722 (3)	C26A—H26A	0.9500
Cl3—C5	1.723 (3)	C26A—C25A	1.3900
Cl4—C6	1.723 (3)	C25A—H25A	0.9500
C1—C2	1.401 (4)	C25A—C24A	1.3900
C1—C6	1.394 (4)	C24A—H24A	0.9500
C2—C3	1.402 (4)	C24A—C23A	1.3900
C3—C4	1.397 (4)	C23A—H23A	0.9500
C4—C5	1.393 (4)	C23A—C22A	1.3900
C5—C6	1.402 (4)	C22A—H22A	0.9500
I3—C7	2.094 (3)	C13B—C18B	1.3900
I4—C10	2.088 (3)	C13B—C14B	1.3900
Cl5—C8	1.719 (3)	C13B—C19B	1.498 (9)
Cl6—C9	1.727 (3)	C18B—H18B	0.9500
Cl7—C11	1.720 (3)	C18B—C17B	1.3900
Cl8—C12	1.723 (3)	C17B—H17B	0.9500
C7—C8	1.397 (4)	C17B—C16B	1.3900
C7—C12	1.396 (4)	C16B—H16B	0.9500
C8—C9	1.397 (4)	C16B—C15B	1.3900
C9—C10	1.396 (4)	C15B—H15B	0.9500
C10—C11	1.396 (4)	C15B—C14B	1.3900
C11—C12	1.401 (4)	C14B—H14B	0.9500
C13A—C18A	1.3900	C19B—H19B	0.9500
C13A—C14A	1.3900	C19B—C20B	1.342 (11)
C13A—C19A	1.494 (8)	C20B—H20B	0.9500
C18A—H18A	0.9500	C20B—C21B	1.497 (9)
C18A—C17A	1.3900	C21B—C26B	1.3900
C17A—H17A	0.9500	C21B—C22B	1.3900
C17A—C16A	1.3900	C26B—H26B	0.9500
C16A—H16A	0.9500	C26B—C25B	1.3900
C16A—C15A	1.3900	C25B—H25B	0.9500
C15A—H15A	0.9500	C25B—C24B	1.3900
C15A—C14A	1.3900	C24B—H24B	0.9500
C14A—H14A	0.9500	C24B—C23B	1.3900
C19A—H19A	0.9500	C23B—H23B	0.9500
C19A—C20A	1.348 (9)	C23B—C22B	1.3900
C20A—H20A	0.9500	C22B—H22B	0.9500
C2—C1—I1	120.0 (2)	C26A—C21A—C20A	121.0 (5)
C6—C1—I1	120.7 (2)	C26A—C21A—C22A	120.0
C6—C1—C2	119.3 (3)	C22A—C21A—C20A	119.0 (5)

C1—C2—Cl1	120.2 (2)	C21A—C26A—H26A	120.0
C1—C2—C3	120.3 (3)	C25A—C26A—C21A	120.0
C3—C2—Cl1	119.4 (2)	C25A—C26A—H26A	120.0
C2—C3—Cl2	118.8 (2)	C26A—C25A—H25A	120.0
C4—C3—Cl2	120.8 (2)	C26A—C25A—C24A	120.0
C4—C3—C2	120.4 (3)	C24A—C25A—H25A	120.0
C3—C4—I2	120.6 (2)	C25A—C24A—H24A	120.0
C5—C4—I2	120.5 (2)	C23A—C24A—C25A	120.0
C5—C4—C3	118.8 (3)	C23A—C24A—H24A	120.0
C4—C5—Cl3	120.0 (2)	C24A—C23A—H23A	120.0
C4—C5—C6	121.2 (3)	C24A—C23A—C22A	120.0
C6—C5—Cl3	118.9 (2)	C22A—C23A—H23A	120.0
C1—C6—Cl4	120.7 (2)	C21A—C22A—H22A	120.0
C1—C6—C5	119.9 (3)	C23A—C22A—C21A	120.0
C5—C6—Cl4	119.4 (2)	C23A—C22A—H22A	120.0
C8—C7—I3	120.0 (2)	C18B—C13B—C14B	120.0
C12—C7—I3	120.9 (2)	C18B—C13B—C19B	118.8 (5)
C12—C7—C8	119.1 (3)	C14B—C13B—C19B	121.2 (5)
C7—C8—Cl5	120.2 (2)	C13B—C18B—H18B	120.0
C7—C8—C9	120.6 (3)	C17B—C18B—C13B	120.0
C9—C8—Cl5	119.2 (2)	C17B—C18B—H18B	120.0
C8—C9—Cl6	119.0 (2)	C18B—C17B—H17B	120.0
C10—C9—Cl6	120.4 (2)	C18B—C17B—C16B	120.0
C10—C9—C8	120.5 (3)	C16B—C17B—H17B	120.0
C9—C10—I4	120.6 (2)	C17B—C16B—H16B	120.0
C11—C10—I4	120.6 (2)	C15B—C16B—C17B	120.0
C11—C10—C9	118.8 (3)	C15B—C16B—H16B	120.0
C10—C11—Cl7	120.0 (2)	C16B—C15B—H15B	120.0
C10—C11—C12	120.8 (3)	C16B—C15B—C14B	120.0
C12—C11—Cl7	119.2 (2)	C14B—C15B—H15B	120.0
C7—C12—Cl8	120.6 (2)	C13B—C14B—H14B	120.0
C7—C12—C11	120.1 (3)	C15B—C14B—C13B	120.0
C11—C12—Cl8	119.3 (2)	C15B—C14B—H14B	120.0
C18A—C13A—C14A	120.0	C13B—C19B—H19B	116.5
C18A—C13A—C19A	122.1 (4)	C20B—C19B—C13B	127.0 (7)
C14A—C13A—C19A	117.9 (4)	C20B—C19B—H19B	116.5
C13A—C18A—H18A	120.0	C19B—C20B—H20B	116.9
C13A—C18A—C17A	120.0	C19B—C20B—C21B	126.2 (7)
C17A—C18A—H18A	120.0	C21B—C20B—H20B	116.9
C18A—C17A—H17A	120.0	C26B—C21B—C20B	117.7 (6)
C16A—C17A—C18A	120.0	C26B—C21B—C22B	120.0
C16A—C17A—H17A	120.0	C22B—C21B—C20B	122.3 (6)
C17A—C16A—H16A	120.0	C21B—C26B—H26B	120.0
C17A—C16A—C15A	120.0	C21B—C26B—C25B	120.0
C15A—C16A—H16A	120.0	C25B—C26B—H26B	120.0
C16A—C15A—H15A	120.0	C26B—C25B—H25B	120.0
C14A—C15A—C16A	120.0	C24B—C25B—C26B	120.0
C14A—C15A—H15A	120.0	C24B—C25B—H25B	120.0

C13A—C14A—H14A	120.0	C25B—C24B—H24B	120.0
C15A—C14A—C13A	120.0	C25B—C24B—C23B	120.0
C15A—C14A—H14A	120.0	C23B—C24B—H24B	120.0
C13A—C19A—H19A	116.1	C24B—C23B—H23B	120.0
C20A—C19A—C13A	127.7 (6)	C24B—C23B—C22B	120.0
C20A—C19A—H19A	116.1	C22B—C23B—H23B	120.0
C19A—C20A—H20A	116.9	C21B—C22B—H22B	120.0
C19A—C20A—C21A	126.3 (6)	C23B—C22B—C21B	120.0
C21A—C20A—H20A	116.9	C23B—C22B—H22B	120.0

I1—C1—C2—Cl1	0.3 (4)	C10—C11—C12—C7	−0.6 (5)
I1—C1—C2—C3	−178.5 (2)	C12—C7—C8—Cl5	179.8 (2)
I1—C1—C6—Cl4	−1.5 (4)	C12—C7—C8—C9	0.1 (5)
I1—C1—C6—C5	178.6 (2)	C13A—C18A—C17A—C16A	0.0
I2—C4—C5—Cl3	0.1 (4)	C13A—C19A—C20A—C21A	179.1 (7)
I2—C4—C5—C6	179.6 (2)	C18A—C13A—C14A—C15A	0.0
Cl1—C2—C3—Cl2	0.3 (4)	C18A—C13A—C19A—C20A	13.5 (9)
Cl1—C2—C3—C4	−179.3 (2)	C18A—C17A—C16A—C15A	0.0
Cl2—C3—C4—I2	1.0 (4)	C17A—C16A—C15A—C14A	0.0
Cl2—C3—C4—C5	−179.4 (2)	C16A—C15A—C14A—C13A	0.0
Cl3—C5—C6—Cl4	−0.2 (4)	C14A—C13A—C18A—C17A	0.0
Cl3—C5—C6—C1	179.6 (2)	C14A—C13A—C19A—C20A	−166.8 (6)
C1—C2—C3—Cl2	179.1 (2)	C19A—C13A—C18A—C17A	179.7 (7)
C1—C2—C3—C4	−0.5 (4)	C19A—C13A—C14A—C15A	−179.7 (7)
C2—C1—C6—Cl4	179.4 (2)	C19A—C20A—C21A—C26A	−20.1 (8)
C2—C1—C6—C5	−0.4 (5)	C19A—C20A—C21A—C22A	158.7 (5)
C2—C3—C4—I2	−179.4 (2)	C20A—C21A—C26A—C25A	178.8 (6)
C2—C3—C4—C5	0.2 (4)	C20A—C21A—C22A—C23A	−178.8 (6)
C3—C4—C5—Cl3	−179.5 (2)	C21A—C26A—C25A—C24A	0.0
C3—C4—C5—C6	−0.1 (5)	C26A—C21A—C22A—C23A	0.0
C4—C5—C6—Cl4	−179.7 (2)	C26A—C25A—C24A—C23A	0.0
C4—C5—C6—C1	0.2 (5)	C25A—C24A—C23A—C22A	0.0
C6—C1—C2—Cl1	179.4 (2)	C24A—C23A—C22A—C21A	0.0
C6—C1—C2—C3	0.6 (4)	C22A—C21A—C26A—C25A	0.0
I3—C7—C8—Cl5	−0.8 (4)	C13B—C18B—C17B—C16B	0.0
I3—C7—C8—C9	179.5 (2)	C13B—C19B—C20B—C21B	179.4 (8)
I3—C7—C12—Cl8	1.1 (4)	C18B—C13B—C14B—C15B	0.0
I3—C7—C12—C11	−179.3 (2)	C18B—C13B—C19B—C20B	−169.6 (7)
I4—C10—C11—Cl7	−0.2 (4)	C18B—C17B—C16B—C15B	0.0
I4—C10—C11—C12	−179.8 (2)	C17B—C16B—C15B—C14B	0.0
Cl5—C8—C9—Cl6	0.3 (4)	C16B—C15B—C14B—C13B	0.0
Cl5—C8—C9—C10	−179.7 (2)	C14B—C13B—C18B—C17B	0.0
Cl6—C9—C10—I4	0.0 (4)	C14B—C13B—C19B—C20B	11.3 (11)
Cl6—C9—C10—C11	179.6 (2)	C19B—C13B—C18B—C17B	−179.2 (8)
Cl7—C11—C12—Cl8	−0.6 (4)	C19B—C13B—C14B—C15B	179.1 (9)
Cl7—C11—C12—C7	179.8 (2)	C19B—C20B—C21B—C26B	164.2 (6)
C7—C8—C9—Cl6	−180.0 (2)	C19B—C20B—C21B—C22B	−16.8 (10)
C7—C8—C9—C10	0.0 (5)	C20B—C21B—C26B—C25B	179.0 (7)

C8—C7—C12—Cl8	−179.4 (2)	C20B—C21B—C22B—C23B	−179.0 (7)
C8—C7—C12—C11	0.2 (5)	C21B—C26B—C25B—C24B	0.0
C8—C9—C10—I4	−180.0 (2)	C26B—C21B—C22B—C23B	0.0
C8—C9—C10—C11	−0.4 (5)	C26B—C25B—C24B—C23B	0.0
C9—C10—C11—Cl7	−179.7 (2)	C25B—C24B—C23B—C22B	0.0
C9—C10—C11—C12	0.7 (5)	C24B—C23B—C22B—C21B	0.0
C10—C11—C12—Cl8	179.0 (2)	C22B—C21B—C26B—C25B	0.0