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# (3a*S*,4*R*,5*R*,6*S*,7a*R*)-4,5-Dibromo-2-[4-(trifluoromethyl)phenyl]-2,3,3a,4,5,6,7,7a-octahydro-3a,6-epoxy-1*H*-isoindol-1-one: crystal structure and Hirshfeld surface analysis

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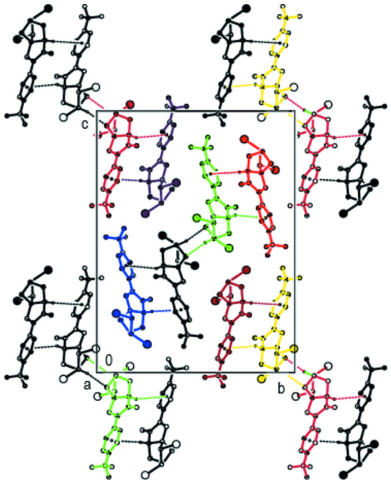
The asymmetric unit of the title compound, $C_{15}H_{12}Br_2F_3NO_2$, consists of two crystallographically independent molecules. In both molecules, the pyrrolidine and tetrahydrofuran rings adopt an envelope conformation. In the crystal, molecule pairs generate centrosymmetric rings with $R_2^2(8)$ motifs linked by C—H···O hydrogen bonds. These pairs of molecules form a tetrameric supramolecular motif, leading to molecular layers parallel to the (100) plane by C—H···$\pi$ and C—Br···$\pi$ interactions. Interlayer van der Waals and interhalogen interactions stabilize molecular packing. The F atoms of the $CF_3$ groups of both molecules are disordered over two sets of sites with refined site occupancies of 0.60 (3)/0.40 (3) and 0.640 (15)/0.360 (15). The most important contributions to the surface contacts of both molecules are from H···H (23.8 and 22.4%), Br···H/H···Br (18.3 and 12.3%), O···H/H···O (14.3 and 9.7%) and F···H/H···F (10.4 and 19.1%) interactions, as concluded from a Hirshfeld surface analysis.

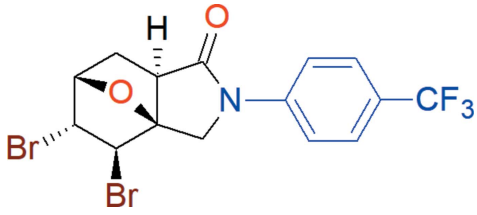


## 1. Chemical context

Isoindoles are important structural units in many natural products and are widely used as drugs and as building-blocks for the construction of new N-containing heterocyclic compounds and functional materials (Nadirova *et al.*, 2019; Zubkov *et al.*, 2011, 2014, 2018). The biological and physical properties of N-heterocycles are dependent on the attached functional groups (Grudova *et al.*, 2020; Zaytsev *et al.*, 2017, 2019, 2020; Asgarova *et al.*, 2019; Khalilov *et al.*, 2011; Yin *et al.*, 2020). Thus, the functionalization of isoindole moieties with non-covalent bond donor/acceptor sites can improve their biological and photophysical properties as well as coordination ability (Wicholas *et al.*, 2006).

On the other hand, non-covalent interactions, such as hydrogen, aerogen, halogen, chalcogen, pnictogen, tetrel and icosagen bonds, as well as $n$–$\pi^*$, $\pi$–$\pi$ stacking, $\pi$–cation, $\pi$–anion and hydrophobic interactions have also attracted much attention recently and have been demonstrated to play a prominent role in synthesis, catalysis, supramolecular chemistry, molecular recognition, biological systems and functional

materials (Asadov *et al.*, 2016; Gurbanov *et al.*, 2017, 2018, 2020; Karmakar *et al.*, 2017; Kopylovich *et al.*, 2011; Ma *et al.*, 2017*a*,*b*; 2020; Mahmudov *et al.*, 2010, 2012, 2013, 2019, 2020; Mizar *et al.*, 2012; Sutradhar *et al.*, 2015, 2016). Halogen bonding is a rather spread phenomenon since halogen atoms or ions can form short non-bonded contacts with electron acceptors, electron donors or be interconnected due to anisotropic charge distribution in halogen atoms (Afkhami *et al.*, 2017; Maharramov *et al.*, 2018, 2019; Mahmoudi *et al.*, 2017, 2019; Shixaliyev *et al.*, 2014). In fact, attachment of isoindoles with non-covalent bond donor or acceptor sites can affect their supramolecular arrangements significantly (Gurbanov *et al.*, 2021).




In a continuation of our work in this direction, we have functionalized a new isoindole, (3a*S*,4*R*,5*R*,6*S*,7a*R*)-4,5-dibromo-2-[4-(trifluoromethyl)phenyl]-2,3,3a,4,5,6,7,7a-octahydro-3a,6-epoxy-1*H*-isoindol-1-one (**1**; Fig. 1), which provides C—Br···$\pi$ halogen bonds as well as C—H···O and C—H···$\pi$ types of intermolecular hydrogen bonds.

## 2. Structural commentary

The asymmetric unit of the title compound (Fig. 2) contains two crystallographically molecules of similar shape, hereafter referred to as molecules *A* (including atom C1) and *B* (including atom C21). The conformational differences between molecules *A* and *B* are highlighted in an overlay diagram shown in Fig. 3. The r.m.s. deviation of the overlay between the molecules *A* and *B* is 0.278 Å.

In both molecules *A* and *B*, the pyrrolidine rings (N2/C1/C3/C3*A*/C7*A* and N22/C21/C23/C23*A*/C27*A*), tetrahydrofuran rings (O8/C3*A*/C4–C6, O8/C3*A*/C6/C7/C7*A* and O28/C23*A*/C24–C26, O28/C23*A*/C26/C27/C27*A*) and six-membered rings (C3*A*/C4–C7/C7*A* and C23*A*/C24–C27/C27*A*), which generate epoxyisoindole moieties (O8/ N2/C1/C3/C3*A*/C4–C7/C7*A* and O28/ N22/C21/C23/C23*A*/C24–C27/C27*A*), are puckered. In molecules *A* and *B*, both tetrahydrofuran rings adopt an envelope conformation with puckering parameters (Cremer & Pople, 1975) $Q(2)$ = 0.580 (3) Å, $\varphi(2)$ = 176.3 (4)° for *A* (O8/C3*A*/C4–C6), $Q(2)$ = 0.547 (3) Å, $\varphi(2)$ = 357.4 (4)° for *A* (O8/C3*A*/C6/C7/C7*A*), and $Q(2)$ = 0.580 (3) Å, $\varphi(2)$ = 180.3 (4)° for *B* (O28/C23*A*/C24–C26) and $Q(2)$ = 0.554 (3) Å, $\varphi(2)$ = 354.2 (4)° for *B* (O28/C23*A*/C26/C27/C27*A*). The five-membered pyrrolidine rings also exhibit an envelope conformation, with a maximum deviation from the mean plane of 0.165 (3) Å at C3*A* [puckering parameters $Q(2)$ = 0.262 (4) Å, $\varphi(2)$ = 281.8 (8)°] for molecule *A* and 0.156 (3) Å at C23*A* [puckering parameters $Q(2)$ = 0.248 (4) Å, $\varphi(2)$ = 291.3 (8)°] for molecule *B*. In both molecules, the six-membered ring has a boat conformation [$Q_T$ = 0.925 (4) Å, $\theta$ = 92.2 (2)°, $\varphi$ = 180.5 (2)° for molecule *A*; $Q_T$ = 0.924 (4) Å, $\theta$ = 91.7 (2)°, $\varphi$ = 177.1 (2)° for molecule *B*].

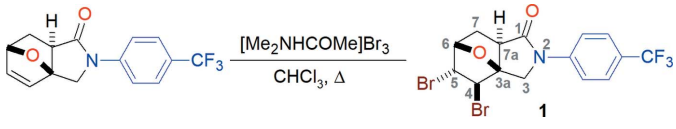



**Figure 1**
Synthesis of (3a*S*,4*R*,5*R*,6*S*,7a*R*)-4,5-dibromo-2-[4-(trifluoromethyl)phenyl]-2,3,3a,4,5,6,7,7a-octahydro-3a,6-epoxy-1*H*-isoindol-1-one (**1**).

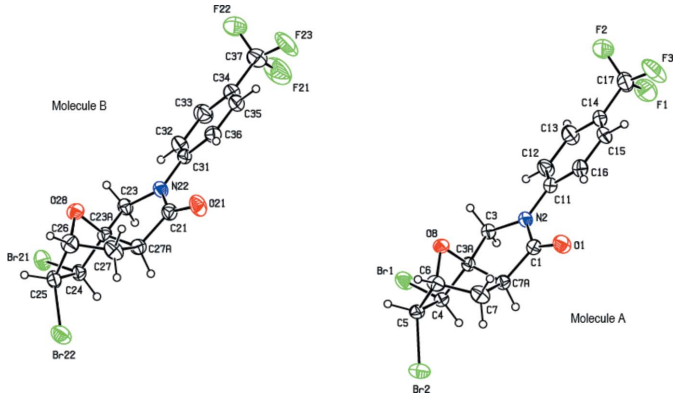



**Figure 2**
The two molecules (*A* and *B*) in the asymmetric unit of the title compound with displacement ellipsoids for the non-hydrogen atoms drawn at the 30% probability level. Hydrogen atoms are shown as spheres of arbitrary radius. The minor components of the disordered $CF_3$ groups were omitted for clarity.

## 3. Supramolecular features

In the crystal, molecules generate centrosymmetric dimers described by $R_2^2(8)$ motifs (Bernstein *et al.*, 1995) by C—H···O

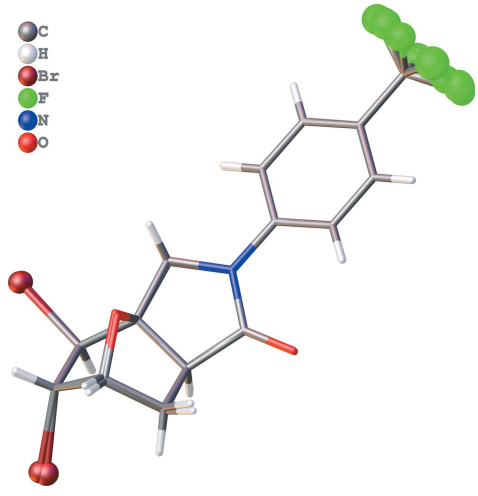



**Figure 3**
Overlay image (*OLEX2*; Dolomanov *et al.*, 2009) of the two molecules (*A* and *B*) in the asymmetric unit of the title compound.

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

*Cg*5 and *Cg*10 are the centroids of the C11–C16 and C31–C36 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5—H5*A*···O8$^{i}$ | 0.98 | 2.57 | 3.342 (4) | 135 |
| C7—H7*A*···Br2 | 0.97 | 2.82 | 3.300 (4) | 112 |
| C16—H16*A*···O1 | 0.93 | 2.26 | 2.853 (4) | 121 |
| C27—H27*A*···Br22 | 0.97 | 2.78 | 3.259 (4) | 111 |
| C36—H36*A*···O21 | 0.93 | 2.28 | 2.856 (5) | 120 |
| C7*A*—H7*AA*···*Cg*10$^{i}$ | 0.98 | 2.94 | 3.741 (4) | 139 |
| C27*A*—H27*C*···*Cg*5$^{i}$ | 0.98 | 2.97 | 3.924 (4) | 166 |

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

hydrogen bonds (Table 1). These pairs of molecules form a tetrameric supramolecular motif, by self-complementary C—H···$\pi$ connections (Fig. 4). Additionally, these building units are self-assembled *via* C—Br···$\pi$ interactions, generating a two-dimensional supramolecular network parallel to the (100) plane (Fig. 5). Interlayer van der Waals and interhalogen interactions stabilize molecular packing.

## 4. Hirshfeld surface analysis

For both molecules *A* and *B*, the intermolecular interactions (Table 2) were quantified using Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) generated. The calculations and visualization were performed using *CrystalExplorer17* (Turner *et al.*, 2017). Fig. 6 shows the Hirshfeld surface of the title compound mapped over $d_{norm}$ in a fixed color scale of −0.2089 (red) to +1.1825 (blue) arbitrary units for molecule *A* and −0.2105 (red) to +1.2372 (blue) arbitrary units for molecule *B*, where the red spots indicate the intermolecular contacts shorter than the van der Waals separations. Fig. 7 shows the full two-dimensional fingerprint plot (Fig. 7*a*) and those delineated into the major contacts: H···H (23.8% for molecule *A* and 22.4% for molecule *B*, Fig. 7*b*) interactions are the major factor in the crystal packing with Br···H/H···Br (18.3% for molecule *A* and 12.3% for

**Table 2**
Summary of short interatomic contacts (Å) in the title compound.

Asterisks indicate symmetry-generated atoms

| Contact | Distance | Symmetry operation |
|---|---|---|
| H5*A*···O8 | 2.57 | $1-x, 1-y, 1-z$ |
| H3*B*···O28 | 2.82 | $x, \frac{3}{2}-y, -\frac{1}{2}+z$ |
| H4*A*···O1 | 2.74 | $-1+x, y, z$ |
| Br2···Br22 | 3.74 | $-x, -\frac{1}{2}+y, \frac{3}{2}-z$ |
| Br2···H26*A* | 2.95 | $1-x, -\frac{1}{2}+y, \frac{3}{2}-z$ |
| H7*AA*···C36 | 2.59 | $1-x, 1-y, 1-z$ |
| *F3*A*···*F23 | 2.90 | $2-x, -\frac{1}{2}+y, \frac{1}{2}-z$ |
| H15*A*···O21 | 2.62 | $2-x, 1-y, 1-z$ |
| *F2*A*···H23*B* | 2.60 | $1+x, \frac{3}{2}-y, -\frac{1}{2}+z$ |
| H23*A*···H36*A* | 2.49 | $-1+x, y, z$ |
| H23*B*···*F2*A* | 2.60 | $-1+x, \frac{3}{2}-y, \frac{1}{2}+z$ |
| Br22···*F23 | 3.48 | $-1+x, \frac{3}{2}-y, \frac{1}{2}+z$ |
| *F22*A*···*F1 | 2.94 | $2-x, \frac{1}{2}+y, \frac{1}{2}-z$ |
| H33*A*···*F21*A* | 2.84 | $1-x, 2-y, 1-z$ |
| *F22*A*···*F22 | 3.09 | $2-x, 2-y, 1-z$ |

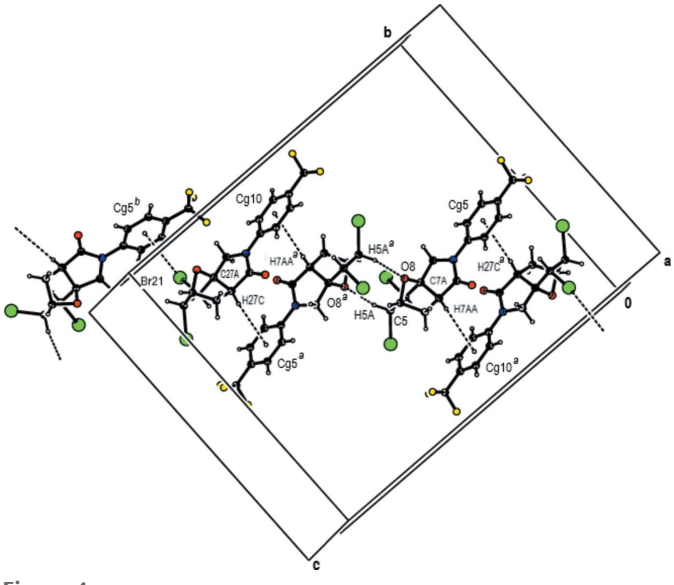



**Figure 4**
A view of the intermolecular C—H···O hydrogen bonds and C—H···$\pi$ and C—Br···$\pi$ interactions in the unit cell of the title compound. Only the major components of the disordered $CF_3$ groups are shown. [Symmetry codes: (*a*) $1-x, 1-y, 1-z$; (*b*) $-1+x, \frac{3}{2}-y, \frac{1}{2}+z$].

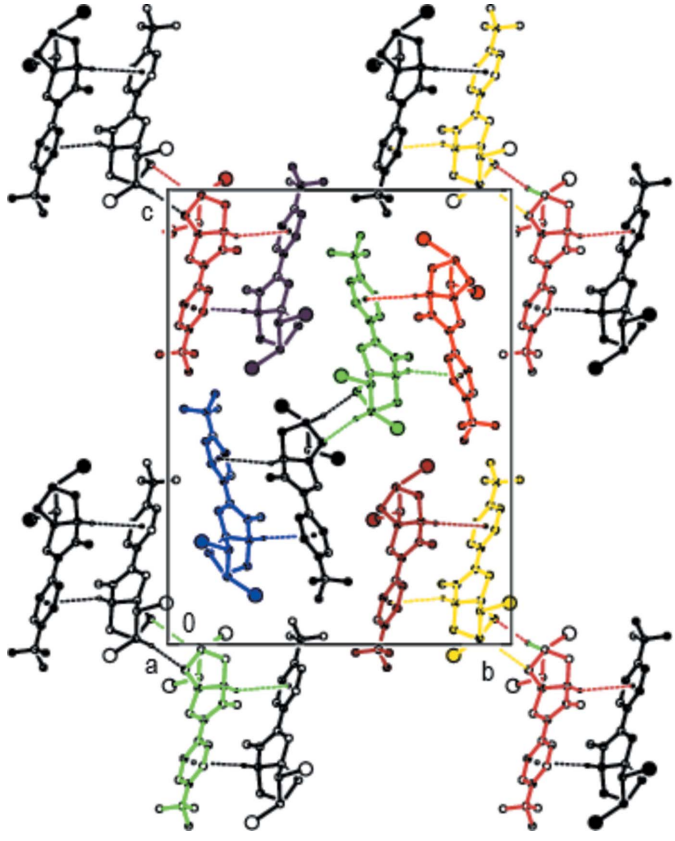
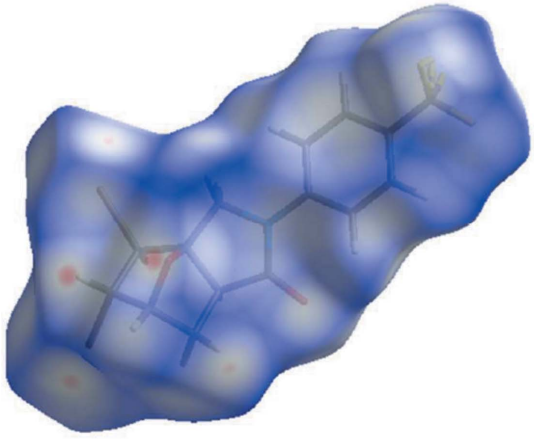



**Figure 5**
A view of the molecular packing of the title compound along the *a* axis. Only the major components of the disordered $CF_3$ groups are shown.

**Table 3**
Percentage contributions of interatomic contacts to the Hirshfeld surface for the molecules *A* and *B* of the title compound.

| Contact | Molecule *A* | Molecule *B* |
|---|---|---|
| H···H | 23.8 | 22.4 |
| Br···H/H···Br | 18.3 | 12.3 |
| O···H/H···O | 14.3 | 9.7 |
| F···H/H···F | 10.4 | 19.1 |
| C···H/H···C | 9.9 | 7.8 |
| F···F | 6.9 | 8.6 |
| Br···F/F···Br | 3.9 | 8.0 |
| Br···C/C···Br | 3.7 | 3.5 |
| Br···Br | 2.4 | 1.6 |
| F···C/C···F | 2.3 | 2.4 |
| Br···O/O···Br | 1.4 | 2.1 |
| Br···N/N···Br | 1.1 | 0.9 |
| O···N/N···O | 0.5 | 0.5 |
| O···C/C···O | 0.5 | 0.4 |
| C···C | 0.3 | 0.3 |
| N···H/H···N | 0.2 | 0.3 |
| N···C/C···N | 0.1 | 0.1 |



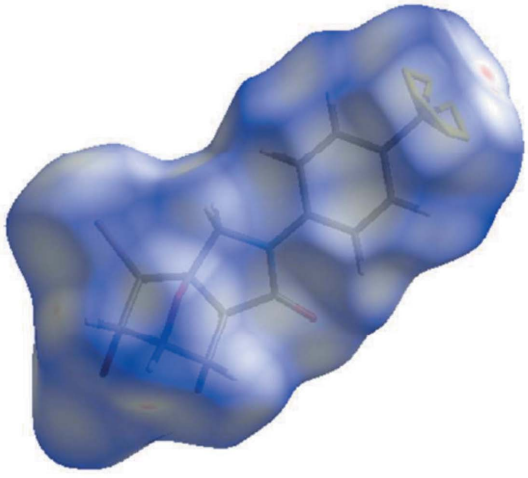




**Figure 6**
Hirshfeld surfaces of molecules *A* and *B* of the title compound mapped with $d_{norm}$.

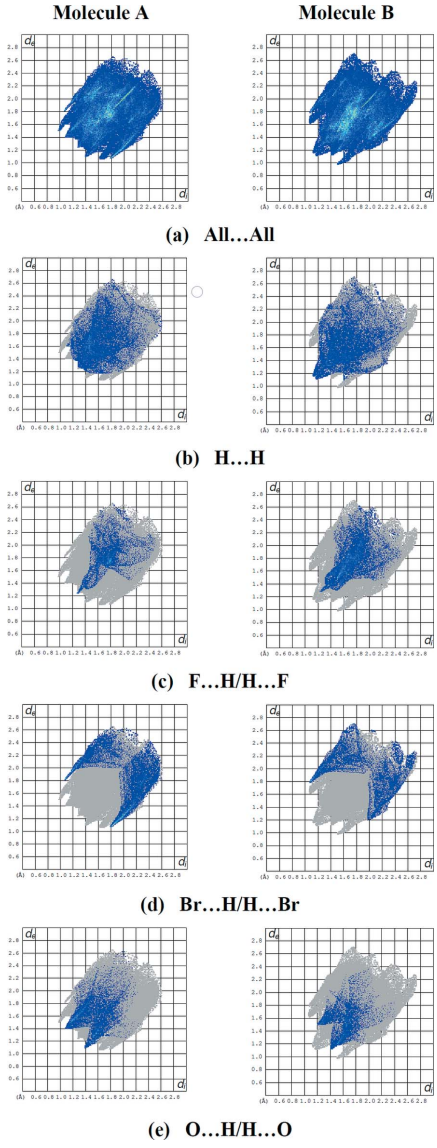



**Figure 7**
The two-dimensional fingerprint plots for molecules *A* and *B* of the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) F···H/H···F, (*d*) Br···H/H···Br and (*e*) O···H/H···O interactions [$d_e$ and $d_i$ represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

molecule *B*, Fig.7*c*), O···H/H···O (14.3% for molecule *A* and 9.7% for molecule *B*, Fig. 7*d*) and F···H/H···F (10.4% for molecule *A* and 19.1% for molecule *B*, Fig. 7*e*) interactions representing the next highest contributions. The percentage contributions of other weak interactions are listed in Table 3. The fact that the same interactions make different contributions to the HS molecules *A* and *B* can be attributed to the different molecular environments of the A and B molecules in the crystalline structure.

## 5. Database survey

A search of the Cambridge Structural Database (CSD version 5.40, update of September 2019; Groom *et al.*, 2016) for

structures having the epoxyisoindole moiety gave eight hits that closely resemble the title compound, *viz.* 4,5-dibromo-6-methyl-2-phenylhexahydro-3a,6-epoxyisoindol-1(4*H*)-one (IMUBIE; Mertsalov *et al.*, 2021*a*), 2-benzyl-4,5-dibromo-hexahydro-3a,6-epoxyisoindol-1(4*H*)-one (OMEMAX; Mertsalov *et al.*, 2021*b*), (3a*R*,6*S*,7a*R*)-7a-chloro-2-[(4-nitrophenyl)sulfonyl]-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole (AGONUH; Temel *et al.*, 2013), (3a*R*,6*S*,7a*R*)-7a-chloro-6-methyl-2-[(4-nitrophenyl)sulfonyl]-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole (TIJMIK; Demircan *et al.*, 2013), 5-chloro-7-methyl-3-[(4-methyl-phenyl)sulfonyl]-10-oxa-3-aza-tricyclo[5.2.1.01,5]dec-8-ene (YAXCIL; Temel *et al.*, 2012), (3a*R*,6*S*,7a*R*)-7a-bromo-2-[(4-methylphenyl)sulfonyl]-1,2,3,6,-7,7a-hexahydro-3a,6-epoxyiso-indole (UPAQEI; Koşar *et al.*, 2011), (3a*R*,6*S*,7a*R*)-7a-bromo-2-methylsulfonyl-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole (ERIVIL; Temel *et al.*, 2011) and *tert*-butyl 3a-chloroper-hydro-2,6a-epoxyoxireno(*e*)iso-indole-5-carboxylate (MIGTIG; Koşar *et al.*, 2007).

In the crystal of IMUBIE, the molecules are linked into dimers by pairs of C—H···O hydrogen bonds, thus generating $R_2^2(18)$ rings. The crystal packing is dominated by H···H, Br···H, H···$\pi$ and Br···$\pi$ interactions. In the crystal structures of OMEMAX, AGONUH, TIJMIK, YAXCIL, UPAQEI and ERIVIL, the molecules are linked by predominantly C—H···O hydrogen bonds describing different hydrogen-bonding pattern connectivities. In OMEMAX, molecules form sheets lying parallel to the (002) plane. These sheets are connected only by weak van der Waals interactions. In the crystal of AGONUH, the molecules are connected in zigzag chains running along the *b*-axis direction. In TIJMIK, two types of C—H···O hydrogen bonds are found, *viz.* $R^2{}_2(20)$ and $R_4^4(26)$ rings, with adjacent rings running parallel to the *ac* plane. Additionally, C—H···O hydrogen bonds form a $C(6)$ chain, linking the molecules in the *b*-axis direction. In the crystal of ERIVIL, the molecules are connected into $R_2^2(8)$ and $R_2^2(14)$ rings along the *b*-axis direction. In MIGTIG, the molecules are linked only by weak van der Waals interactions.

## 6. Synthesis and crystallization

(3a*S*,6*S*,7a*R*)-2-(4-(Trifluoromethyl)phenyl)-2,3,7,7a-tetra-hydro-3a,6-epoxyisoindol-1(6*H*)-one (1.2 mmol) and the brominating agent $[(Me_2NCOMe)_2H]Br_3$ (1.32 mmol) in 3 mL of dry chloroform were heated under reflux for 3–5 h (TLC control, EtOAc–hexane, 1:1). The reaction mixture was poured into $H_2O$ (50 mL), extracted with $CHCl_3$ (3 × 20 mL) and combined organic parts were dried over anhydrous $Na_2SO_4$ and the solvent was evaporated under reduced pressure. Recrystallization of the obtained residue from a hexane–AcOEt mixture gave single crystals suitable for X-ray analysis.

Yield 15%, m.p. > 438 K (decomp.), pale-beige plates. $^1$H NMR (600.2 MHz, $CDCl_3$) $\delta$ 7.79 (*d*, *J* = 8.1 Hz, 2H, H-3, H-5 $H_{arom.}$), 7.64 (*d*, *J* = 8.1 Hz, 2H, H-2, H-6 $H_{arom.}$), 4.78 (*t*, *J* = 5.0 Hz, 1H, H-6), 4.53 (*ddd*, *J* = 4.0 Hz, *J* = 1.3 Hz, *J* = 2.3 Hz, 1H, H-5), 4.26 (*t*, *J* = 2.3 Hz, 1H, H-4), 4.13 (*dd*, *J* = 11.6 Hz, *J* = 1.7 Hz, 1H), 4.09 (*dd*, *J* = 11.6 Hz, *J* = 1.7 Hz, 1H, H-3), 2.99 (*dd*, *J* = 4.5 Hz, *J* = 9.1 Hz, 1H, H-7a), 2.83 (*ddd*, *J* = 1.7 Hz, *J* = 9.1 Hz, *J* = 13.1 Hz, 1H, H-7B), 2.35–2.31 (*m*, 1H, H-7A). $^{13}$C NMR (150.9 MHz, $CDCl_3$) $\delta$ 172.7, 141.6, 126.7 (*q*, *J* = 33.2 Hz, 1C), 126.2 (*q*, *J* = 2.9 Hz, 2C), 123.8 (*J* = 271.6 Hz, 1C), 119.4 (2C), 88.7, 80.1, 55.5, 53.8, 50.5, 49.7, 30.9. $^{19}$F NMR (564.7 MHz, $CDCl_3$) $\delta$ −62.1. IR (KBr): 1703 (NC=O). MS (ESI): *m*/*z* = 456 [*M* + H$^+$]. Analysis calculated for $C_{15}H_{12}Br_2F_3NO_2$: C 39.59%, H 2.66%, N 3.08%. Found: C 39.55%, H 2.61%, N 3.20%.

**Table 4**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{15}H_{12}Br_2F_3NO_2$ |
| $M_r$ | 455.08 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 296 |
| *a*, *b*, *c* (Å) | 6.6543 (2), 18.9031 (5), 25.1995 (7) |
| $\beta$ (°) | 97.132 (2) |
| *V* (Å$^3$) | 3145.24 (15) |
| *Z* | 8 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 5.19 |
| Crystal size (mm) | 0.44 × 0.12 × 0.04 |
| | |
| Data collection | |
| Diffractometer | Bruker *KAPPA* APEXII area-detector |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2013) |
| $T_{min}$, $T_{max}$ | 0.704, 0.819 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 44884, 7199, 4255 |
| $R_{int}$ | 0.057 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.650 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.038, 0.077, 1.00 |
| No. of reflections | 7199 |
| No. of parameters | 471 |
| No. of restraints | 204 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.52, −0.44 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

## 7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. All C-bound H atoms were placed at calculated positions using a riding model, with aromatic C—H = 0.93–0.98 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C). The F atoms of the trifluoromethyl groups ($CF_3$) of both molecules are disordered over two sets of sites with refined site occupancies of 0.60 (3)/0.40 (3) for molecule *A* and 0.640 (15)/0.360 (15) for molecule *B*. The major and minor components of the disordered $CF_3$ groups of molecules *A* and *B* were restrained to have approximately equal C—F distances by use of the *SHELXL* SADI instruction. The anisotropies of the F1, F2, F3, F1*A*, F2*A*, F3*A*, F21, F22, F23, F21*A*, F22*A* and F23*A* atoms were restrained with ISOR 0.01 0.02 in *SHELXL* (Sheldrick, 2015*b*). Six outliers ($\bar{3}$ 1 4, $\bar{1}$ 2 11, $\bar{3}$ 2 5, $\bar{2}$ 7 7, $\bar{1}$ 4 7 and $\bar{1}$ 10 25) were omitted in the final refinement.

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# supporting information

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## (3a*S*,4*R*,5*R*,6*S*,7a*R*)-4,5-Dibromo-2-[4-(trifluoromethyl)-phenyl]-2,3,3a,4,5,6,7,7a-octahydro-3a,6-epoxy-1*H*-isoindol-1-one: crystal structure and Hirshfeld surface analysis

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### Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

### (3a*S*,4*R*,5*R*,6*S*,7a*R*)-4,5-Dibromo-2-[4-(trifluoromethyl)phenyl]-2,3,3a,4,5,6,7,7a-octahydro-3a,6-epoxy-1*H*-isoindol-1-one

*Crystal data*

$C_{15}H_{12}Br_2F_3NO_2$
$M_r$ = 455.08
Monoclinic, $P2_1/c$
$a$ = 6.6543 (2) Å
$b$ = 18.9031 (5) Å
$c$ = 25.1995 (7) Å
$\beta$ = 97.132 (2)°
$V$ = 3145.24 (15) Å$^3$
$Z$ = 8
$F(000)$ = 1776
$D_x$ = 1.922 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 6983 reflections
$\theta$ = 3.1–22.1°
$\mu$ = 5.19 mm$^{-1}$
$T$ = 296 K
Plate, light beige
0.44 × 0.12 × 0.04 mm

*Data collection*

Bruker KAPPA APEXII area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
$T_{min}$ = 0.704, $T_{max}$ = 0.819
44884 measured reflections
7199 independent reflections
4255 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 4.2°
$h$ = −8→8
$k$ = −24→24
$l$ = −32→32

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.077
$S$ = 1.00
7199 reflections
471 parameters
204 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0254P)^2 + 2.067P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.52$ e Å$^{-3}$
$\Delta\rho_{min} = -0.44$ e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Br1 | 0.04969 (6) | 0.49524 (2) | 0.40882 (2) | 0.05936 (12) | |
| Br2 | 0.16433 (6) | 0.33168 (2) | 0.52432 (2) | 0.05972 (13) | |
| F1 | 0.8250 (14) | 0.4392 (8) | 0.1004 (3) | 0.100 (3) | 0.60 (3) |
| F2 | 0.984 (3) | 0.5243 (3) | 0.1380 (4) | 0.097 (3) | 0.60 (3) |
| F3 | 1.1221 (17) | 0.4233 (8) | 0.1395 (5) | 0.105 (4) | 0.60 (3) |
| F1A | 0.8229 (18) | 0.4756 (13) | 0.1027 (6) | 0.099 (5) | 0.40 (3) |
| F2A | 1.084 (3) | 0.5104 (9) | 0.1523 (7) | 0.100 (5) | 0.40 (3) |
| F3A | 1.056 (3) | 0.4043 (6) | 0.1284 (6) | 0.082 (4) | 0.40 (3) |
| O1 | 0.7970 (4) | 0.29869 (13) | 0.36728 (11) | 0.0602 (7) | |
| O8 | 0.5397 (3) | 0.44953 (12) | 0.44391 (9) | 0.0477 (6) | |
| N2 | 0.6066 (4) | 0.39552 (14) | 0.33412 (11) | 0.0394 (7) | |
| C1 | 0.6561 (5) | 0.33992 (18) | 0.36860 (14) | 0.0423 (8) | |
| C3 | 0.4324 (5) | 0.43625 (18) | 0.34806 (13) | 0.0417 (8) | |
| H3A | 0.311584 | 0.426135 | 0.323570 | 0.050* | |
| H3B | 0.459315 | 0.486670 | 0.347699 | 0.050* | |
| C3A | 0.4104 (5) | 0.41102 (17) | 0.40351 (13) | 0.0368 (8) | |
| C4 | 0.2098 (5) | 0.41007 (17) | 0.42722 (13) | 0.0394 (8) | |
| H4A | 0.131785 | 0.367487 | 0.416059 | 0.047* | |
| C5 | 0.2862 (5) | 0.40741 (18) | 0.48724 (13) | 0.0436 (8) | |
| H5A | 0.254387 | 0.452572 | 0.503380 | 0.052* | |
| C6 | 0.5167 (5) | 0.4022 (2) | 0.48785 (14) | 0.0489 (9) | |
| H6A | 0.592991 | 0.417081 | 0.521802 | 0.059* | |
| C7 | 0.5857 (5) | 0.3323 (2) | 0.46770 (15) | 0.0548 (10) | |
| H7A | 0.526303 | 0.292812 | 0.484771 | 0.066* | |
| H7B | 0.732082 | 0.328072 | 0.473085 | 0.066* | |
| C7A | 0.5045 (5) | 0.33729 (17) | 0.40819 (13) | 0.0387 (8) | |
| H7AA | 0.402046 | 0.300829 | 0.398258 | 0.046* | |
| C11 | 0.6955 (5) | 0.41029 (17) | 0.28750 (14) | 0.0399 (8) | |
| C12 | 0.5936 (6) | 0.4528 (2) | 0.24827 (16) | 0.0553 (10) | |
| H12A | 0.468838 | 0.472055 | 0.253387 | 0.066* | |
| C13 | 0.6754 (6) | 0.4671 (2) | 0.20159 (16) | 0.0613 (11) | |
| H13A | 0.604994 | 0.495703 | 0.175597 | 0.074* | |
| C14 | 0.8598 (6) | 0.43931 (19) | 0.19327 (15) | 0.0498 (9) | |
| C15 | 0.9620 (5) | 0.39722 (19) | 0.23196 (15) | 0.0486 (9) | |
| H15A | 1.087012 | 0.378300 | 0.226660 | 0.058* | |
| C16 | 0.8817 (5) | 0.38265 (18) | 0.27862 (14) | 0.0468 (9) | |

| | | | | | |
|---|---|---|---|---|---|
| H16A | 0.952961 | 0.353997 | 0.304433 | 0.056* | |
| C17 | 0.9517 (7) | 0.4566 (2) | 0.14398 (18) | 0.0672 (12) | |
| Br21 | −0.02652 (5) | 0.90131 (2) | 0.77414 (2) | 0.05796 (12) | |
| Br22 | 0.19224 (7) | 0.74494 (2) | 0.89213 (2) | 0.07068 (14) | |
| F21 | 0.6437 (15) | 0.8625 (7) | 0.4491 (3) | 0.138 (4) | 0.640 (15) |
| F22 | 0.7980 (19) | 0.9531 (3) | 0.4818 (4) | 0.113 (3) | 0.640 (15) |
| F23 | 0.9516 (12) | 0.8560 (6) | 0.4812 (3) | 0.116 (3) | 0.640 (15) |
| F21A | 0.674 (3) | 0.9420 (7) | 0.4653 (6) | 0.111 (5) | 0.360 (15) |
| F22A | 0.9709 (17) | 0.9064 (12) | 0.4937 (5) | 0.137 (6) | 0.360 (15) |
| F23A | 0.751 (3) | 0.8377 (5) | 0.4539 (4) | 0.094 (4) | 0.360 (15) |
| O21 | 0.7477 (4) | 0.73028 (14) | 0.72019 (11) | 0.0656 (8) | |
| O28 | 0.4682 (3) | 0.87970 (12) | 0.79846 (9) | 0.0481 (6) | |
| N22 | 0.5250 (4) | 0.81952 (15) | 0.69035 (11) | 0.0414 (7) | |
| C21 | 0.6025 (5) | 0.76761 (19) | 0.72515 (15) | 0.0451 (9) | |
| C23 | 0.3412 (5) | 0.85182 (19) | 0.70647 (13) | 0.0422 (8) | |
| H23A | 0.220656 | 0.833540 | 0.685316 | 0.051* | |
| H23B | 0.344086 | 0.902874 | 0.702787 | 0.051* | |
| C23A | 0.3480 (4) | 0.83071 (17) | 0.76374 (13) | 0.0372 (8) | |
| C24 | 0.1603 (5) | 0.82315 (18) | 0.79201 (14) | 0.0425 (8) | |
| H24A | 0.093727 | 0.777509 | 0.783839 | 0.051* | |
| C25 | 0.2563 (5) | 0.82648 (19) | 0.85095 (14) | 0.0481 (9) | |
| H25A | 0.207680 | 0.869136 | 0.867414 | 0.058* | |
| C26 | 0.4823 (5) | 0.8359 (2) | 0.84539 (15) | 0.0538 (10) | |
| H26A | 0.558598 | 0.858168 | 0.876756 | 0.065* | |
| C27 | 0.5823 (5) | 0.7695 (2) | 0.82783 (15) | 0.0578 (11) | |
| H27A | 0.555775 | 0.729042 | 0.849561 | 0.069* | |
| H27B | 0.727365 | 0.775539 | 0.828410 | 0.069* | |
| C27A | 0.4739 (5) | 0.76308 (18) | 0.77028 (14) | 0.0431 (8) | |
| H27C | 0.386791 | 0.721131 | 0.766510 | 0.052* | |
| C31 | 0.5911 (5) | 0.83652 (18) | 0.64070 (14) | 0.0418 (8) | |
| C32 | 0.4639 (6) | 0.8728 (2) | 0.60261 (15) | 0.0556 (10) | |
| H32A | 0.336348 | 0.886497 | 0.610202 | 0.067* | |
| C33 | 0.5228 (7) | 0.8889 (2) | 0.55368 (17) | 0.0674 (12) | |
| H33A | 0.435143 | 0.913322 | 0.528468 | 0.081* | |
| C34 | 0.7117 (7) | 0.8691 (2) | 0.54186 (17) | 0.0624 (11) | |
| C35 | 0.8395 (6) | 0.8327 (2) | 0.57932 (17) | 0.0597 (11) | |
| H35A | 0.966193 | 0.818608 | 0.571272 | 0.072* | |
| C36 | 0.7822 (5) | 0.81668 (19) | 0.62877 (16) | 0.0508 (9) | |
| H36A | 0.870853 | 0.792753 | 0.654043 | 0.061* | |
| C37 | 0.7765 (9) | 0.8866 (3) | 0.4889 (2) | 0.0852 (15) | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0517 (2) | 0.0598 (3) | 0.0702 (3) | 0.01235 (19) | 0.0221 (2) | 0.0094 (2) |
| Br2 | 0.0562 (2) | 0.0703 (3) | 0.0529 (3) | −0.0180 (2) | 0.00743 (19) | 0.0129 (2) |
| F1 | 0.139 (5) | 0.110 (7) | 0.053 (4) | −0.014 (4) | 0.028 (3) | 0.003 (4) |
| F2 | 0.146 (7) | 0.066 (4) | 0.090 (5) | −0.004 (4) | 0.059 (5) | 0.013 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| F3 | 0.098 (5) | 0.135 (7) | 0.095 (6) | 0.033 (5) | 0.060 (4) | 0.032 (5) |
| F1A | 0.106 (6) | 0.124 (9) | 0.073 (6) | 0.007 (6) | 0.033 (5) | 0.039 (6) |
| F2A | 0.111 (8) | 0.104 (8) | 0.093 (7) | −0.056 (6) | 0.048 (6) | −0.011 (5) |
| F3A | 0.123 (8) | 0.063 (5) | 0.075 (6) | 0.000 (5) | 0.065 (6) | −0.016 (4) |
| O1 | 0.0612 (16) | 0.0520 (16) | 0.0717 (19) | 0.0192 (13) | 0.0251 (14) | 0.0135 (14) |
| O8 | 0.0473 (14) | 0.0514 (15) | 0.0459 (15) | −0.0230 (11) | 0.0111 (11) | −0.0137 (12) |
| N2 | 0.0396 (15) | 0.0386 (16) | 0.0414 (17) | 0.0037 (13) | 0.0107 (13) | −0.0023 (14) |
| C1 | 0.0430 (19) | 0.038 (2) | 0.046 (2) | −0.0013 (16) | 0.0085 (17) | −0.0035 (17) |
| C3 | 0.0440 (19) | 0.038 (2) | 0.045 (2) | 0.0012 (15) | 0.0123 (16) | −0.0014 (16) |
| C3A | 0.0372 (17) | 0.038 (2) | 0.0360 (19) | −0.0049 (15) | 0.0076 (15) | −0.0069 (15) |
| C4 | 0.0397 (18) | 0.0359 (19) | 0.043 (2) | −0.0047 (15) | 0.0074 (16) | −0.0032 (16) |
| C5 | 0.047 (2) | 0.044 (2) | 0.041 (2) | −0.0137 (16) | 0.0122 (16) | −0.0071 (17) |
| C6 | 0.043 (2) | 0.069 (3) | 0.034 (2) | −0.0185 (19) | −0.0001 (16) | −0.0061 (19) |
| C7 | 0.042 (2) | 0.071 (3) | 0.051 (2) | 0.0065 (19) | 0.0047 (18) | 0.010 (2) |
| C7A | 0.0369 (18) | 0.0373 (19) | 0.042 (2) | −0.0022 (15) | 0.0069 (15) | −0.0033 (16) |
| C11 | 0.0433 (19) | 0.0356 (19) | 0.042 (2) | −0.0004 (16) | 0.0106 (16) | −0.0053 (16) |
| C12 | 0.056 (2) | 0.054 (2) | 0.060 (3) | 0.0161 (19) | 0.023 (2) | 0.010 (2) |
| C13 | 0.073 (3) | 0.058 (3) | 0.056 (3) | 0.022 (2) | 0.021 (2) | 0.014 (2) |
| C14 | 0.062 (2) | 0.042 (2) | 0.049 (2) | 0.0024 (18) | 0.022 (2) | −0.0051 (18) |
| C15 | 0.046 (2) | 0.054 (2) | 0.049 (2) | 0.0034 (18) | 0.0199 (18) | −0.0035 (19) |
| C16 | 0.048 (2) | 0.046 (2) | 0.046 (2) | 0.0053 (17) | 0.0057 (17) | −0.0022 (18) |
| C17 | 0.085 (3) | 0.061 (3) | 0.060 (3) | 0.011 (3) | 0.029 (3) | −0.001 (3) |
| Br21 | 0.0449 (2) | 0.0658 (3) | 0.0640 (3) | 0.01529 (19) | 0.01001 (18) | −0.0037 (2) |
| Br22 | 0.0775 (3) | 0.0783 (3) | 0.0609 (3) | 0.0063 (2) | 0.0271 (2) | 0.0142 (2) |
| F21 | 0.152 (6) | 0.201 (8) | 0.066 (4) | −0.033 (5) | 0.033 (4) | −0.014 (5) |
| F22 | 0.168 (7) | 0.079 (4) | 0.105 (5) | −0.015 (4) | 0.070 (5) | 0.016 (3) |
| F23 | 0.133 (5) | 0.135 (6) | 0.098 (4) | 0.027 (4) | 0.084 (4) | 0.020 (4) |
| F21A | 0.140 (9) | 0.106 (8) | 0.096 (7) | 0.033 (6) | 0.058 (6) | 0.041 (6) |
| F22A | 0.127 (8) | 0.169 (11) | 0.126 (8) | −0.033 (7) | 0.058 (6) | 0.029 (7) |
| F23A | 0.155 (9) | 0.073 (6) | 0.060 (5) | 0.006 (6) | 0.044 (6) | −0.004 (4) |
| O21 | 0.0596 (16) | 0.0704 (19) | 0.071 (2) | 0.0285 (14) | 0.0227 (14) | 0.0036 (15) |
| O28 | 0.0453 (13) | 0.0506 (15) | 0.0469 (15) | −0.0105 (11) | −0.0005 (11) | −0.0058 (12) |
| N22 | 0.0339 (14) | 0.0492 (18) | 0.0421 (17) | 0.0020 (13) | 0.0088 (13) | −0.0051 (14) |
| C21 | 0.0384 (19) | 0.047 (2) | 0.050 (2) | 0.0017 (17) | 0.0064 (17) | −0.0056 (18) |
| C23 | 0.0351 (17) | 0.049 (2) | 0.043 (2) | 0.0041 (15) | 0.0061 (15) | −0.0030 (17) |
| C23A | 0.0323 (16) | 0.0379 (19) | 0.041 (2) | −0.0039 (15) | 0.0022 (15) | −0.0074 (16) |
| C24 | 0.0396 (18) | 0.042 (2) | 0.047 (2) | 0.0026 (15) | 0.0097 (16) | −0.0066 (17) |
| C25 | 0.054 (2) | 0.050 (2) | 0.043 (2) | 0.0045 (18) | 0.0140 (17) | −0.0065 (18) |
| C26 | 0.051 (2) | 0.068 (3) | 0.040 (2) | −0.005 (2) | −0.0041 (18) | −0.006 (2) |
| C27 | 0.042 (2) | 0.079 (3) | 0.052 (3) | 0.013 (2) | 0.0056 (18) | 0.009 (2) |
| C27A | 0.0360 (18) | 0.042 (2) | 0.052 (2) | 0.0030 (15) | 0.0069 (16) | 0.0021 (17) |
| C31 | 0.0422 (19) | 0.044 (2) | 0.040 (2) | −0.0074 (16) | 0.0101 (16) | −0.0095 (17) |
| C32 | 0.053 (2) | 0.066 (3) | 0.050 (3) | 0.009 (2) | 0.015 (2) | 0.001 (2) |
| C33 | 0.076 (3) | 0.069 (3) | 0.059 (3) | 0.005 (2) | 0.019 (2) | 0.007 (2) |
| C34 | 0.081 (3) | 0.055 (3) | 0.056 (3) | −0.015 (2) | 0.028 (2) | −0.010 (2) |
| C35 | 0.057 (2) | 0.059 (3) | 0.068 (3) | −0.012 (2) | 0.028 (2) | −0.017 (2) |
| C36 | 0.042 (2) | 0.057 (2) | 0.055 (2) | −0.0074 (17) | 0.0092 (18) | −0.0097 (19) |
| C37 | 0.113 (5) | 0.080 (4) | 0.069 (4) | −0.019 (4) | 0.038 (3) | −0.003 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C4 | 1.954 (3) | Br21—C24 | 1.947 (3) |
| Br2—C5 | 1.941 (3) | Br22—C25 | 1.935 (4) |
| F1—F1A | 0.691 (15) | F21—F23A | 0.852 (11) |
| F1—C17 | 1.341 (7) | F21—C37 | 1.332 (7) |
| F1—F3A | 1.738 (15) | F21—F21A | 1.564 (13) |
| F2—F2A | 0.764 (14) | F22—F21A | 0.899 (13) |
| F2—C17 | 1.308 (7) | F22—C37 | 1.280 (7) |
| F2—F1A | 1.596 (14) | F22—F22A | 1.452 (14) |
| F3—F3A | 0.610 (16) | F23—F22A | 1.007 (15) |
| F3—C17 | 1.314 (7) | F23—C37 | 1.337 (7) |
| F3—F2A | 1.703 (13) | F23—F23A | 1.463 (13) |
| F1A—C17 | 1.313 (9) | F21A—C37 | 1.347 (9) |
| F2A—C17 | 1.345 (9) | F22A—C37 | 1.338 (9) |
| F3A—C17 | 1.295 (9) | F23A—C37 | 1.275 (9) |
| O1—C1 | 1.223 (4) | O21—C21 | 1.215 (4) |
| O8—C3A | 1.446 (4) | O28—C26 | 1.437 (4) |
| O8—C6 | 1.446 (4) | O28—C23A | 1.445 (4) |
| N2—C1 | 1.377 (4) | N22—C21 | 1.373 (4) |
| N2—C11 | 1.407 (4) | N22—C31 | 1.414 (4) |
| N2—C3 | 1.470 (4) | N22—C23 | 1.469 (4) |
| C1—C7A | 1.505 (4) | C21—C27A | 1.508 (5) |
| C3—C3A | 1.501 (4) | C23—C23A | 1.492 (5) |
| C3—H3A | 0.9700 | C23—H23A | 0.9700 |
| C3—H3B | 0.9700 | C23—H23B | 0.9700 |
| C3A—C7A | 1.527 (4) | C23A—C24 | 1.520 (4) |
| C3A—C4 | 1.529 (4) | C23A—C27A | 1.526 (4) |
| C4—C5 | 1.535 (5) | C24—C25 | 1.543 (5) |
| C4—H4A | 0.9800 | C24—H24A | 0.9800 |
| C5—C6 | 1.536 (5) | C25—C26 | 1.538 (5) |
| C5—H5A | 0.9800 | C25—H25A | 0.9800 |
| C6—C7 | 1.508 (5) | C26—C27 | 1.511 (5) |
| C6—H6A | 0.9800 | C26—H26A | 0.9800 |
| C7—C7A | 1.532 (5) | C27—C27A | 1.542 (5) |
| C7—H7A | 0.9700 | C27—H27A | 0.9700 |
| C7—H7B | 0.9700 | C27—H27B | 0.9700 |
| C7A—H7AA | 0.9800 | C27A—H27C | 0.9800 |
| C11—C12 | 1.385 (5) | C31—C32 | 1.380 (5) |
| C11—C16 | 1.388 (4) | C31—C36 | 1.394 (5) |
| C12—C13 | 1.382 (5) | C32—C33 | 1.374 (5) |
| C12—H12A | 0.9300 | C32—H32A | 0.9300 |
| C13—C14 | 1.375 (5) | C33—C34 | 1.379 (6) |
| C13—H13A | 0.9300 | C33—H33A | 0.9300 |
| C14—C15 | 1.372 (5) | C34—C35 | 1.374 (6) |
| C14—C17 | 1.488 (5) | C34—C37 | 1.489 (6) |
| C15—C16 | 1.379 (5) | C35—C36 | 1.381 (5) |
| C15—H15A | 0.9300 | C35—H35A | 0.9300 |

| | | | |
|---|---|---|---|
| C16—H16A | 0.9300 | C36—H36A | 0.9300 |
| | | | |
| F1A—F1—C17 | 72.7 (11) | F23A—F21—C37 | 67.4 (8) |
| F1A—F1—F3A | 111.7 (13) | F23A—F21—F21A | 114.4 (10) |
| C17—F1—F3A | 47.6 (5) | C37—F21—F21A | 54.7 (5) |
| F2A—F2—C17 | 76.0 (9) | F21A—F22—C37 | 74.0 (8) |
| F2A—F2—F1A | 123.5 (11) | F21A—F22—F22A | 127.7 (11) |
| C17—F2—F1A | 52.6 (4) | C37—F22—F22A | 58.3 (5) |
| F3A—F3—C17 | 74.8 (13) | F22A—F23—C37 | 68.0 (7) |
| F3A—F3—F2A | 122.7 (14) | F22A—F23—F23A | 116.4 (9) |
| C17—F3—F2A | 51.0 (4) | C37—F23—F23A | 54.0 (4) |
| F1—F1A—C17 | 77.2 (11) | F22—F21A—C37 | 66.0 (7) |
| F1—F1A—F2 | 127.1 (13) | F22—F21A—F21 | 115.1 (10) |
| C17—F1A—F2 | 52.4 (5) | C37—F21A—F21 | 53.8 (5) |
| F2—F2A—C17 | 70.6 (9) | F23—F22A—C37 | 67.8 (7) |
| F2—F2A—F3 | 112.5 (12) | F23—F22A—F22 | 116.3 (9) |
| C17—F2A—F3 | 49.4 (4) | C37—F22A—F22 | 54.5 (5) |
| F3—F3A—C17 | 78.2 (12) | F21—F23A—C37 | 74.6 (8) |
| F3—F3A—F1 | 121.1 (15) | F21—F23A—F23 | 129.5 (10) |
| C17—F3A—F1 | 49.9 (5) | C37—F23A—F23 | 58.0 (5) |
| C3A—O8—C6 | 96.7 (2) | C26—O28—C23A | 96.0 (2) |
| C1—N2—C11 | 125.8 (3) | C21—N22—C31 | 126.4 (3) |
| C1—N2—C3 | 112.5 (3) | C21—N22—C23 | 112.3 (3) |
| C11—N2—C3 | 121.4 (3) | C31—N22—C23 | 120.8 (3) |
| O1—C1—N2 | 126.4 (3) | O21—C21—N22 | 126.1 (3) |
| O1—C1—C7A | 125.2 (3) | O21—C21—C27A | 125.3 (3) |
| N2—C1—C7A | 108.4 (3) | N22—C21—C27A | 108.6 (3) |
| N2—C3—C3A | 103.1 (3) | N22—C23—C23A | 103.3 (3) |
| N2—C3—H3A | 111.1 | N22—C23—H23A | 111.1 |
| C3A—C3—H3A | 111.1 | C23A—C23—H23A | 111.1 |
| N2—C3—H3B | 111.1 | N22—C23—H23B | 111.1 |
| C3A—C3—H3B | 111.1 | C23A—C23—H23B | 111.1 |
| H3A—C3—H3B | 109.1 | H23A—C23—H23B | 109.1 |
| O8—C3A—C3 | 112.2 (3) | O28—C23A—C23 | 111.2 (3) |
| O8—C3A—C7A | 101.7 (2) | O28—C23A—C24 | 101.6 (3) |
| C3—C3A—C7A | 106.0 (3) | C23—C23A—C24 | 123.4 (3) |
| O8—C3A—C4 | 101.7 (2) | O28—C23A—C27A | 102.5 (2) |
| C3—C3A—C4 | 124.0 (3) | C23—C23A—C27A | 106.2 (3) |
| C7A—C3A—C4 | 109.2 (3) | C24—C23A—C27A | 110.0 (3) |
| C3A—C4—C5 | 100.8 (2) | C23A—C24—C25 | 100.4 (3) |
| C3A—C4—Br1 | 112.0 (2) | C23A—C24—Br21 | 111.0 (2) |
| C5—C4—Br1 | 111.4 (2) | C25—C24—Br21 | 111.6 (2) |
| C3A—C4—H4A | 110.8 | C23A—C24—H24A | 111.1 |
| C5—C4—H4A | 110.8 | C25—C24—H24A | 111.1 |
| Br1—C4—H4A | 110.8 | Br21—C24—H24A | 111.1 |
| C4—C5—C6 | 102.7 (3) | C26—C25—C24 | 102.1 (3) |
| C4—C5—Br2 | 113.0 (2) | C26—C25—Br22 | 115.1 (3) |
| C6—C5—Br2 | 115.1 (2) | C24—C25—Br22 | 113.0 (2) |

| | | | |
|---|---|---|---|
| C4—C5—H5A | 108.6 | C26—C25—H25A | 108.8 |
| C6—C5—H5A | 108.6 | C24—C25—H25A | 108.8 |
| Br2—C5—H5A | 108.6 | Br22—C25—H25A | 108.8 |
| O8—C6—C7 | 102.6 (3) | O28—C26—C27 | 102.9 (3) |
| O8—C6—C5 | 98.8 (3) | O28—C26—C25 | 100.2 (3) |
| C7—C6—C5 | 113.5 (3) | C27—C26—C25 | 113.7 (3) |
| O8—C6—H6A | 113.5 | O28—C26—H26A | 113.0 |
| C7—C6—H6A | 113.5 | C27—C26—H26A | 113.0 |
| C5—C6—H6A | 113.5 | C25—C26—H26A | 113.0 |
| C6—C7—C7A | 101.0 (3) | C26—C27—C27A | 99.7 (3) |
| C6—C7—H7A | 111.6 | C26—C27—H27A | 111.8 |
| C7A—C7—H7A | 111.6 | C27A—C27—H27A | 111.8 |
| C6—C7—H7B | 111.6 | C26—C27—H27B | 111.8 |
| C7A—C7—H7B | 111.6 | C27A—C27—H27B | 111.8 |
| H7A—C7—H7B | 109.4 | H27A—C27—H27B | 109.5 |
| C1—C7A—C3A | 102.8 (3) | C21—C27A—C23A | 103.1 (3) |
| C1—C7A—C7 | 117.8 (3) | C21—C27A—C27 | 117.5 (3) |
| C3A—C7A—C7 | 102.9 (3) | C23A—C27A—C27 | 102.8 (3) |
| C1—C7A—H7AA | 110.9 | C21—C27A—H27C | 110.9 |
| C3A—C7A—H7AA | 110.9 | C23A—C27A—H27C | 110.9 |
| C7—C7A—H7AA | 110.9 | C27—C27A—H27C | 110.9 |
| C12—C11—C16 | 118.1 (3) | C32—C31—C36 | 118.7 (3) |
| C12—C11—N2 | 119.5 (3) | C32—C31—N22 | 119.8 (3) |
| C16—C11—N2 | 122.4 (3) | C36—C31—N22 | 121.5 (3) |
| C13—C12—C11 | 120.8 (3) | C33—C32—C31 | 121.0 (4) |
| C13—C12—H12A | 119.6 | C33—C32—H32A | 119.5 |
| C11—C12—H12A | 119.6 | C31—C32—H32A | 119.5 |
| C14—C13—C12 | 120.6 (4) | C32—C33—C34 | 120.2 (4) |
| C14—C13—H13A | 119.7 | C32—C33—H33A | 119.9 |
| C12—C13—H13A | 119.7 | C34—C33—H33A | 119.9 |
| C15—C14—C13 | 119.1 (3) | C35—C34—C33 | 119.4 (4) |
| C15—C14—C17 | 120.2 (3) | C35—C34—C37 | 120.2 (4) |
| C13—C14—C17 | 120.7 (4) | C33—C34—C37 | 120.4 (5) |
| C14—C15—C16 | 120.8 (3) | C34—C35—C36 | 120.8 (4) |
| C14—C15—H15A | 119.6 | C34—C35—H35A | 119.6 |
| C16—C15—H15A | 119.6 | C36—C35—H35A | 119.6 |
| C15—C16—C11 | 120.7 (3) | C35—C36—C31 | 119.8 (4) |
| C15—C16—H16A | 119.6 | C35—C36—H36A | 120.1 |
| C11—C16—H16A | 119.6 | C31—C36—H36A | 120.1 |
| F3A—C17—F2 | 127.6 (8) | F23A—C37—F22 | 128.3 (7) |
| F3A—C17—F1A | 106.8 (9) | F22—C37—F21 | 107.7 (7) |
| F2—C17—F1A | 75.0 (7) | F23A—C37—F23 | 68.1 (6) |
| F2—C17—F3 | 107.6 (6) | F22—C37—F23 | 106.8 (6) |
| F1A—C17—F3 | 123.2 (9) | F21—C37—F23 | 104.5 (6) |
| F3A—C17—F1 | 82.5 (8) | F23A—C37—F22A | 107.8 (8) |
| F2—C17—F1 | 103.9 (6) | F22—C37—F22A | 67.3 (7) |
| F3—C17—F1 | 105.9 (6) | F21—C37—F22A | 134.9 (8) |
| F3A—C17—F2A | 105.1 (7) | F23A—C37—F21A | 104.0 (8) |

| | | | |
|---|---|---|---|
| F1A—C17—F2A | 105.5 (7) | F21—C37—F21A | 71.4 (7) |
| F3—C17—F2A | 79.7 (7) | F23—C37—F21A | 132.3 (7) |
| F1—C17—F2A | 130.3 (8) | F22A—C37—F21A | 104.6 (8) |
| F3A—C17—C14 | 112.0 (7) | F23A—C37—C34 | 115.6 (6) |
| F2—C17—C14 | 113.7 (5) | F22—C37—C34 | 113.3 (5) |
| F1A—C17—C14 | 115.2 (7) | F21—C37—C34 | 111.1 (5) |
| F3—C17—C14 | 114.5 (6) | F23—C37—C34 | 112.9 (5) |
| F1—C17—C14 | 110.4 (5) | F22A—C37—C34 | 111.6 (7) |
| F2A—C17—C14 | 111.5 (7) | F21A—C37—C34 | 112.5 (7) |
| | | | |
| F3A—F1—F1A—C17 | −27.9 (13) | F22A—F22—F21A—C37 | 24.2 (13) |
| C17—F1—F1A—F2 | 16.9 (19) | C37—F22—F21A—F21 | −22.7 (10) |
| F3A—F1—F1A—F2 | −11 (3) | F22A—F22—F21A—F21 | 1 (2) |
| F2A—F2—F1A—F1 | 8 (4) | F23A—F21—F21A—F22 | −7 (2) |
| C17—F2—F1A—F1 | −21 (2) | C37—F21—F21A—F22 | 25.9 (12) |
| F2A—F2—F1A—C17 | 29.2 (19) | F23A—F21—F21A—C37 | −33.1 (13) |
| F1A—F2—F2A—C17 | −23.6 (14) | F23A—F23—F22A—C37 | 24.6 (9) |
| C17—F2—F2A—F3 | 26.8 (11) | C37—F23—F22A—F22 | −25.6 (9) |
| F1A—F2—F2A—F3 | 3 (2) | F23A—F23—F22A—F22 | −1.0 (16) |
| F3A—F3—F2A—F2 | −11 (4) | F21A—F22—F22A—F23 | 2 (2) |
| C17—F3—F2A—F2 | −34.1 (15) | C37—F22—F22A—F23 | 29.5 (10) |
| F3A—F3—F2A—C17 | 23 (3) | F21A—F22—F22A—C37 | −27.6 (16) |
| F2A—F3—F3A—C17 | −18 (2) | F21A—F21—F23A—C37 | 28.9 (11) |
| C17—F3—F3A—F1 | 26.6 (18) | C37—F21—F23A—F23 | −19.7 (14) |
| F2A—F3—F3A—F1 | 8 (4) | F21A—F21—F23A—F23 | 9 (2) |
| F1A—F1—F3A—F3 | 2 (4) | F22A—F23—F23A—F21 | −6 (2) |
| C17—F1—F3A—F3 | −35 (3) | C37—F23—F23A—F21 | 22.6 (16) |
| F1A—F1—F3A—C17 | 37 (2) | F22A—F23—F23A—C37 | −28.5 (11) |
| C11—N2—C1—O1 | 7.5 (6) | C31—N22—C21—O21 | 4.1 (6) |
| C3—N2—C1—O1 | −178.0 (3) | C23—N22—C21—O21 | 176.5 (3) |
| C11—N2—C1—C7A | −171.5 (3) | C31—N22—C21—C27A | −174.4 (3) |
| C3—N2—C1—C7A | 3.0 (4) | C23—N22—C21—C27A | −2.1 (4) |
| C1—N2—C3—C3A | 13.8 (4) | C21—N22—C23—C23A | 17.2 (4) |
| C11—N2—C3—C3A | −171.4 (3) | C31—N22—C23—C23A | −169.9 (3) |
| C6—O8—C3A—C3 | −167.2 (3) | C26—O28—C23A—C23 | −166.9 (3) |
| C6—O8—C3A—C7A | −54.4 (3) | C26—O28—C23A—C24 | 60.0 (3) |
| C6—O8—C3A—C4 | 58.3 (3) | C26—O28—C23A—C27A | −53.8 (3) |
| N2—C3—C3A—O8 | 85.4 (3) | N22—C23—C23A—O28 | 85.8 (3) |
| N2—C3—C3A—C7A | −24.7 (3) | N22—C23—C23A—C24 | −153.2 (3) |
| N2—C3—C3A—C4 | −152.0 (3) | N22—C23—C23A—C27A | −25.0 (3) |
| O8—C3A—C4—C5 | −32.6 (3) | O28—C23A—C24—C25 | −36.2 (3) |
| C3—C3A—C4—C5 | −159.7 (3) | C23—C23A—C24—C25 | −161.6 (3) |
| C7A—C3A—C4—C5 | 74.4 (3) | C27A—C23A—C24—C25 | 71.8 (3) |
| O8—C3A—C4—Br1 | 85.9 (3) | O28—C23A—C24—Br21 | 81.9 (3) |
| C3—C3A—C4—Br1 | −41.2 (4) | C23—C23A—C24—Br21 | −43.5 (4) |
| C7A—C3A—C4—Br1 | −167.1 (2) | C27A—C23A—C24—Br21 | −170.0 (2) |
| C3A—C4—C5—C6 | −3.6 (3) | C23A—C24—C25—C26 | 0.4 (3) |
| Br1—C4—C5—C6 | −122.6 (2) | Br21—C24—C25—C26 | −117.3 (3) |

| | | | |
|---|---|---|---|
| C3A—C4—C5—Br2 | −128.3 (2) | C23A—C24—C25—Br22 | −123.9 (2) |
| Br1—C4—C5—Br2 | 112.7 (2) | Br21—C24—C25—Br22 | 118.5 (2) |
| C3A—O8—C6—C7 | 57.2 (3) | C23A—O28—C26—C27 | 58.8 (3) |
| C3A—O8—C6—C5 | −59.4 (3) | C23A—O28—C26—C25 | −58.6 (3) |
| C4—C5—C6—O8 | 38.5 (3) | C24—C25—C26—O28 | 35.6 (3) |
| Br2—C5—C6—O8 | 161.8 (2) | Br22—C25—C26—O28 | 158.5 (2) |
| C4—C5—C6—C7 | −69.5 (4) | C24—C25—C26—C27 | −73.4 (4) |
| Br2—C5—C6—C7 | 53.8 (4) | Br22—C25—C26—C27 | 49.4 (4) |
| O8—C6—C7—C7A | −36.4 (3) | O28—C26—C27—C27A | −39.5 (3) |
| C5—C6—C7—C7A | 69.2 (3) | C25—C26—C27—C27A | 67.9 (4) |
| O1—C1—C7A—C3A | 162.7 (3) | O21—C21—C27A—C23A | 167.8 (3) |
| N2—C1—C7A—C3A | −18.2 (3) | N22—C21—C27A—C23A | −13.6 (4) |
| O1—C1—C7A—C7 | 50.5 (5) | O21—C21—C27A—C27 | 55.6 (5) |
| N2—C1—C7A—C7 | −130.5 (3) | N22—C21—C27A—C27 | −125.8 (3) |
| O8—C3A—C7A—C1 | −91.0 (3) | O28—C23A—C27A—C21 | −92.9 (3) |
| C3—C3A—C7A—C1 | 26.4 (3) | C23—C23A—C27A—C21 | 23.9 (3) |
| C4—C3A—C7A—C1 | 162.1 (3) | C24—C23A—C27A—C21 | 159.6 (3) |
| O8—C3A—C7A—C7 | 31.9 (3) | O28—C23A—C27A—C27 | 29.7 (3) |
| C3—C3A—C7A—C7 | 149.3 (3) | C23—C23A—C27A—C27 | 146.5 (3) |
| C4—C3A—C7A—C7 | −75.0 (3) | C24—C23A—C27A—C27 | −77.8 (3) |
| C6—C7—C7A—C1 | 114.7 (3) | C26—C27—C27A—C21 | 117.8 (3) |
| C6—C7—C7A—C3A | 2.5 (3) | C26—C27—C27A—C23A | 5.4 (3) |
| C1—N2—C11—C12 | 160.0 (3) | C21—N22—C31—C32 | 159.3 (3) |
| C3—N2—C11—C12 | −14.1 (5) | C23—N22—C31—C32 | −12.5 (5) |
| C1—N2—C11—C16 | −18.8 (5) | C21—N22—C31—C36 | −19.9 (5) |
| C3—N2—C11—C16 | 167.1 (3) | C23—N22—C31—C36 | 168.3 (3) |
| C16—C11—C12—C13 | 0.2 (6) | C36—C31—C32—C33 | 0.3 (6) |
| N2—C11—C12—C13 | −178.7 (3) | N22—C31—C32—C33 | −178.9 (4) |
| C11—C12—C13—C14 | −0.1 (6) | C31—C32—C33—C34 | −0.1 (6) |
| C12—C13—C14—C15 | 0.0 (6) | C32—C33—C34—C35 | 0.4 (6) |
| C12—C13—C14—C17 | −177.8 (4) | C32—C33—C34—C37 | −179.8 (4) |
| C13—C14—C15—C16 | 0.1 (6) | C33—C34—C35—C36 | −0.9 (6) |
| C17—C14—C15—C16 | 177.8 (4) | C37—C34—C35—C36 | 179.3 (4) |
| C14—C15—C16—C11 | 0.0 (5) | C34—C35—C36—C31 | 1.1 (6) |
| C12—C11—C16—C15 | −0.1 (5) | C32—C31—C36—C35 | −0.8 (5) |
| N2—C11—C16—C15 | 178.7 (3) | N22—C31—C36—C35 | 178.3 (3) |
| F3—F3A—C17—F2 | 48 (3) | F21—F23A—C37—F22 | −67.6 (15) |
| F1—F3A—C17—F2 | −101.8 (9) | F23—F23A—C37—F22 | 94.5 (9) |
| F3—F3A—C17—F1A | 132 (2) | F23—F23A—C37—F21 | 162.1 (13) |
| F1—F3A—C17—F1A | −18.0 (9) | F21—F23A—C37—F23 | −162.1 (13) |
| F1—F3A—C17—F3 | −150 (2) | F21—F23A—C37—F22A | −142.4 (11) |
| F3—F3A—C17—F1 | 150 (2) | F23—F23A—C37—F22A | 19.7 (8) |
| F3—F3A—C17—F2A | 20 (2) | F21—F23A—C37—F21A | −31.8 (13) |
| F1—F3A—C17—F2A | −129.8 (8) | F23—F23A—C37—F21A | 130.3 (7) |
| F3—F3A—C17—C14 | −101 (2) | F21—F23A—C37—C34 | 92.0 (12) |
| F1—F3A—C17—C14 | 109.0 (6) | F23—F23A—C37—C34 | −105.8 (6) |
| F2A—F2—C17—F3A | −55.3 (17) | F21A—F22—C37—F23A | 62.3 (14) |
| F1A—F2—C17—F3A | 99.9 (10) | F22A—F22—C37—F23A | −95.3 (10) |

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| F2A—F2—C17—F1A | −155.2 (17) | F21A—F22—C37—F21 | 25.5 (12) |
| F2A—F2—C17—F3 | −34.5 (16) | F22A—F22—C37—F21 | −132.0 (8) |
| F1A—F2—C17—F3 | 120.7 (9) | F21A—F22—C37—F23 | 137.3 (11) |
| F2A—F2—C17—F1 | −146.5 (14) | F22A—F22—C37—F23 | −20.3 (8) |
| F1A—F2—C17—F1 | 8.7 (10) | F21A—F22—C37—F22A | 157.6 (13) |
| F1A—F2—C17—F2A | 155.2 (17) | F22A—F22—C37—F21A | −157.6 (13) |
| F2A—F2—C17—C14 | 93.5 (15) | F21A—F22—C37—C34 | −97.7 (12) |
| F1A—F2—C17—C14 | −111.3 (8) | F22A—F22—C37—C34 | 104.7 (8) |
| F1—F1A—C17—F3A | 38 (2) | F21A—F21—C37—F23A | −147.4 (13) |
| F2—F1A—C17—F3A | −125.4 (8) | F23A—F21—C37—F22 | 130.4 (12) |
| F1—F1A—C17—F2 | 163 (2) | F21A—F21—C37—F22 | −17.0 (8) |
| F1—F1A—C17—F3 | 61 (2) | F23A—F21—C37—F23 | 17.1 (12) |
| F2—F1A—C17—F3 | −101.5 (8) | F21A—F21—C37—F23 | −130.3 (7) |
| F2—F1A—C17—F1 | −163 (2) | F23A—F21—C37—F22A | 55.1 (16) |
| F1—F1A—C17—F2A | 149.1 (17) | F21A—F21—C37—F22A | −92.3 (11) |
| F2—F1A—C17—F2A | −13.9 (9) | F23A—F21—C37—F21A | 147.4 (13) |
| F1—F1A—C17—C14 | −87.5 (19) | F23A—F21—C37—C34 | −105.0 (12) |
| F2—F1A—C17—C14 | 109.5 (6) | F21A—F21—C37—C34 | 107.6 (7) |
| F2A—F3—C17—F3A | 160 (2) | F22A—F23—C37—F23A | 152.5 (11) |
| F3A—F3—C17—F2 | −142 (2) | F22A—F23—C37—F22 | 27.3 (10) |
| F2A—F3—C17—F2 | 18.5 (9) | F23A—F23—C37—F22 | −125.3 (8) |
| F3A—F3—C17—F1A | −58 (2) | F22A—F23—C37—F21 | 141.3 (10) |
| F2A—F3—C17—F1A | 101.8 (9) | F23A—F23—C37—F21 | −11.3 (8) |
| F3A—F3—C17—F1 | −31 (2) | F23A—F23—C37—F22A | −152.5 (11) |
| F2A—F3—C17—F1 | 129.1 (8) | F22A—F23—C37—F21A | 63.3 (13) |
| F3A—F3—C17—F2A | −160 (2) | F23A—F23—C37—F21A | −89.2 (12) |
| F3A—F3—C17—C14 | 91 (2) | F22A—F23—C37—C34 | −97.9 (10) |
| F2A—F3—C17—C14 | −109.0 (7) | F23A—F23—C37—C34 | 109.6 (7) |
| F1A—F1—C17—F3A | −144 (2) | F23—F22A—C37—F23A | −26.7 (11) |
| F1A—F1—C17—F2 | −17 (2) | F22—F22A—C37—F23A | 124.9 (8) |
| F3A—F1—C17—F2 | 127.0 (8) | F23—F22A—C37—F22 | −151.6 (10) |
| F3A—F1—C17—F1A | 144 (2) | F23—F22A—C37—F21 | −58.8 (13) |
| F1A—F1—C17—F3 | −130.2 (19) | F22—F22A—C37—F21 | 92.8 (11) |
| F3A—F1—C17—F3 | 13.7 (10) | F22—F22A—C37—F23 | 151.6 (10) |
| F1A—F1—C17—F2A | −40 (2) | F23—F22A—C37—F21A | −136.9 (9) |
| F3A—F1—C17—F2A | 103.5 (10) | F22—F22A—C37—F21A | 14.6 (9) |
| F1A—F1—C17—C14 | 105.3 (18) | F23—F22A—C37—C34 | 101.2 (9) |
| F3A—F1—C17—C14 | −110.7 (7) | F22—F22A—C37—C34 | −107.2 (6) |
| F2—F2A—C17—F3A | 137.6 (14) | F22—F21A—C37—F23A | −134.3 (11) |
| F3—F2A—C17—F3A | −9.1 (11) | F21—F21A—C37—F23A | 20.0 (8) |
| F3—F2A—C17—F2 | −146.7 (15) | F21—F21A—C37—F22 | 154.3 (12) |
| F2—F2A—C17—F1A | 24.9 (17) | F22—F21A—C37—F21 | −154.3 (12) |
| F3—F2A—C17—F1A | −121.8 (9) | F22—F21A—C37—F23 | −61.4 (14) |
| F2—F2A—C17—F3 | 146.7 (15) | F21—F21A—C37—F23 | 92.9 (10) |
| F2—F2A—C17—F1 | 44.6 (17) | F22—F21A—C37—F22A | −21.3 (13) |
| F3—F2A—C17—F1 | −102.1 (9) | F21—F21A—C37—F22A | 133.0 (8) |
| F2—F2A—C17—C14 | −100.8 (14) | F22—F21A—C37—C34 | 99.9 (10) |
| F3—F2A—C17—C14 | 112.4 (7) | F21—F21A—C37—C34 | −105.8 (6) |

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| C15—C14—C17—F3A | 35.6 (11) | C35—C34—C37—F23A | 83.5 (11) |
| C13—C14—C17—F3A | −146.7 (10) | C33—C34—C37—F23A | −96.2 (11) |
| C15—C14—C17—F2 | −118.1 (9) | C35—C34—C37—F22 | −113.7 (8) |
| C13—C14—C17—F2 | 59.6 (10) | C33—C34—C37—F22 | 66.5 (9) |
| C15—C14—C17—F1A | 157.9 (13) | C35—C34—C37—F21 | 124.9 (8) |
| C13—C14—C17—F1A | −24.4 (14) | C33—C34—C37—F21 | −54.9 (9) |
| C15—C14—C17—F3 | 6.2 (11) | C35—C34—C37—F23 | 7.9 (8) |
| C13—C14—C17—F3 | −176.1 (10) | C33—C34—C37—F23 | −171.9 (7) |
| C15—C14—C17—F1 | 125.6 (8) | C35—C34—C37—F22A | −40.1 (13) |
| C13—C14—C17—F1 | −56.8 (9) | C33—C34—C37—F22A | 140.1 (12) |
| C15—C14—C17—F2A | −81.9 (13) | C35—C34—C37—F21A | −157.2 (11) |
| C13—C14—C17—F2A | 95.8 (13) | C33—C34—C37—F21A | 23.0 (12) |

*Hydrogen-bond geometry (Å, º)*

*Cg*5 and *Cg*10 are the centroids of the C11–C16 and C31–C36 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5—H5*A*···O8$^{i}$ | 0.98 | 2.57 | 3.342 (4) | 135 |
| C7—H7*A*···Br2 | 0.97 | 2.82 | 3.300 (4) | 112 |
| C16—H16*A*···O1 | 0.93 | 2.26 | 2.853 (4) | 121 |
| C27—H27*A*···Br22 | 0.97 | 2.78 | 3.259 (4) | 111 |
| C36—H36*A*···O21 | 0.93 | 2.28 | 2.856 (5) | 120 |
| C7*A*—H7*AA*···*Cg*10$^{i}$ | 0.98 | 2.94 | 3.741 (4) | 139 |
| C27*A*—H27*C*···*Cg*5$^{i}$ | 0.98 | 2.97 | 3.924 (4) | 166 |

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