Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Supramolecular networks in (9-fluoro-4*H*-chromeno[4,3-*c*]isoxazol-3-yl)-methanol and its 9-chloro analogue at 100 K[1]

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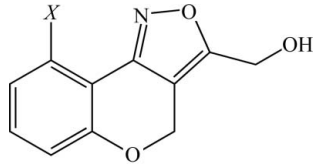
Received 23 February 2012
Accepted 5 June 2012
Online 1 July 2012

The title compounds, (9-fluoro-4*H*-chromeno[4,3-*c*]isoxazol-3-yl)methanol, $C_{11}H_8FNO_3$, (I), and (9-chloro-4*H*-chromeno-[4,3-*c*]isoxazol-3-yl)methanol, $C_{11}H_8ClNO_3$, (II), crystallize in the orthorhombic space group *Pbca* with $Z' = 1$ and the triclinic space group $P\overline{1}$ with $Z' = 6$, respectively. The simple replacement of F by Cl in the main molecular scaffold of (I) and (II) results in significant differences in the intermolecular interaction patterns and a corresponding change in the point-group symmetry from D_{2h} to $C_i = S_2$. These striking differences are manifested through the presence of C—H···F and the absence of O—H···O and C—H···O interactions in (I), and the absence of C—H···Cl and the presence of O—H···O and C—H···O interactions in (II). However, the geometry of the synthons formed by the O—H···N and O—H···*X* (*X* = F or Cl) interactions observed in the constitution of the supramolecular networks of both (I) and (II) remains similar. Also, C—H···O interactions are not preferred in the presence of F in (I), while they are much preferred in the presence of Cl in (II).

Comment

Isoxazole derivatives have interesting biological and medicinal applications (Lin *et al.*,1996, Hu *et al.*, 2004). Leflunomide {systematic name: 5-methyl-*N*-[4-(trifluoromethyl)phenyl]-isoxazole-4-carboxamide} is an isoxazole drug used for the treatment of rheumatoid arthritis (Rozman *et al.*, 2002). The study of fluorine-, bromine- and chlorine-substituted leflunomide metabolite analogues has shown that the presence of an F atom at the 2-position of the phenyl ring disrupts the intermolecular hydrogen bonding that is observed for the other derivatives, due to differences in the crystal packing for these molecules (Venkatachalam *et al.*, 2005). Since interactions involving halogens are known to contribute to characteristic supramolecular synthons (Pedireddi *et al.*, 1992; Desiraju *et al.*, 1993), the present description of the crystal structures of (9-fluoro-4*H*-chromeno[4,3-*c*]isoxazol-3-yl)methanol, (I), and its 9-chloro analogue, (II), may contribute to the development of crystal-engineering strategies. Some of the recent reports of structures that are relevant to the present study are: 3-(3-chlorophenyl)-1-methyl-3,3a,4,9b-tetrahydro-1*H*-chromeno[4,3-*c*]isoxazole-3a-carbonitrile (Swaminathan *et al.*, 2011*a*), its 1-methyl-3-*p*-tolyl-substituted analogue (Gangadharan *et al.*, 2011), and 1-methyl-3-(2-methylphenyl)-3,3a,4,9b-tetrahydro-1*H*-chromeno[4,3-*c*][1,2]oxazole-3a-carbonitrile (Swaminathan *et al.*, 2011*b*).



(I) X = F
(II) X = Cl

The simple replacement of F by Cl lowers the point-group symmetry of the crystal structure from D_{2h} in (I) to $C_i = S_2$ in (II). The unit cell of (II) presents a complex picture, with six molecules in its asymmetric unit (*A*–*F*), each differing from the others in conformation and related by pseudo-translations and pseudo-inversion centres. There are pseudo-inversion centres at [0.34 (2), 0.50 (1), 0.16 (1)] between molecules *B* and *F*, at [0.83 (3), 0.50 (2), 0.17 (1)] between molecules *D* and *E*, and at [0.67 (3), 0.50 (2), 0.37 (1)] between molecules *C* and *E*. The pseudo-translations are [−0.33 (3), −0.01 (2), 0.33 (2)], relating molecules *C* and *D*, and [−0.33 (1), −0.01 (1), 0.33 (1)], relating molecules *A* and *B*. The molecular structures of (I) and (II) are shown in Figs. 1 and 2, and selected bond lengths, bond angles and torsion angles are listed in Tables 1 and 3, respectively.

The geometric parameters of the 4*H*-chromeno[4,3-*c*]-isoxazole rings of (I) and (II) are comparable with those reported for similar structures retrieved from the Cambridge

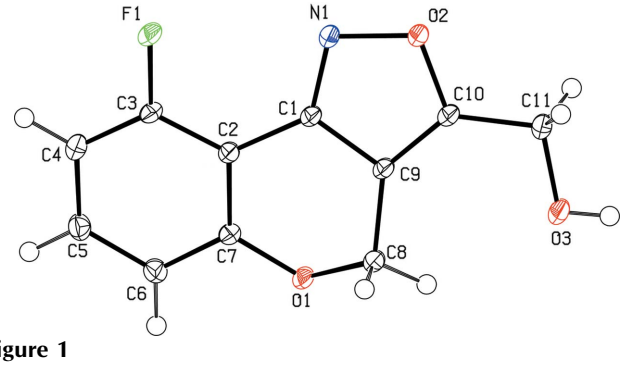


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

[1] This paper is dedicated to the memory of Professor R. K. Rajaram.

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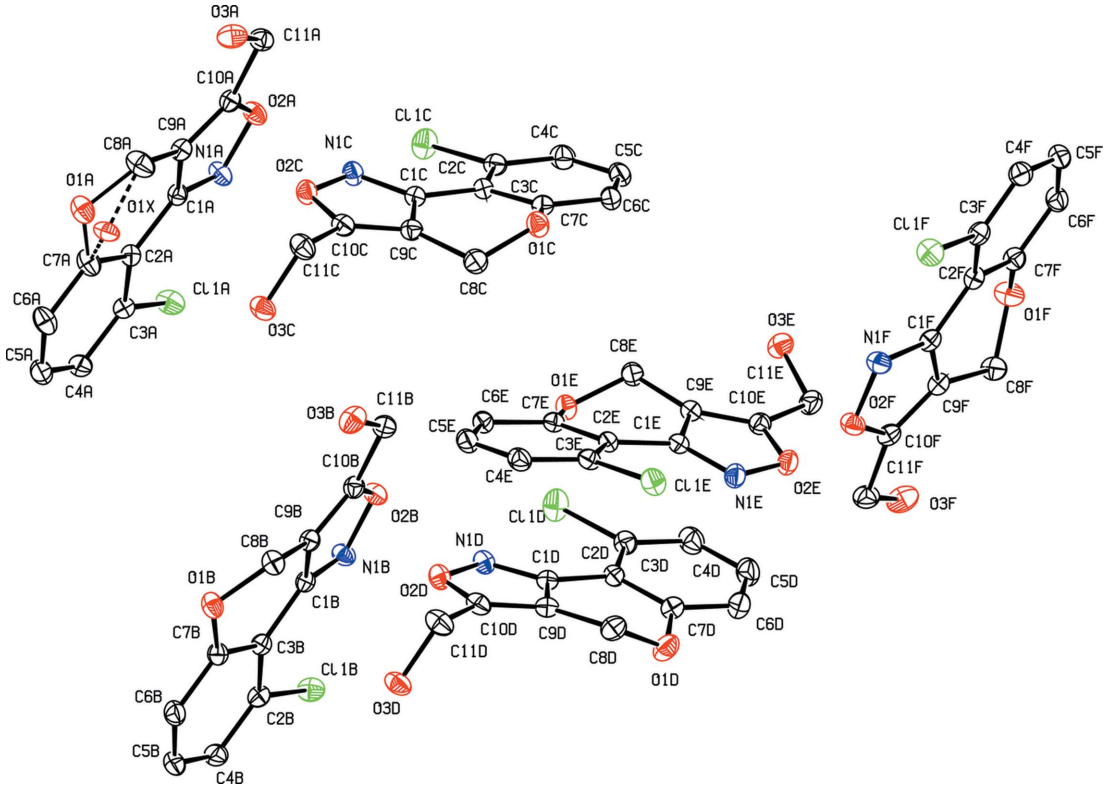

Figure 2
The six molecules in the asymmetric unit of (II), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed lines indicate the minor disorder component of atom O1 in molecule *A*. H atoms have been omitted for clarity.

Structural Database (Version 5.32: Allen, 2002). However, in (I), the O1—C8 [1.4526 (14) Å; Raihan *et al.*, 2010; Liaskopoulos *et al.*, 2007] and O3—C11 [1.4107 (15) Å] bond lengths differ significantly from the respective mean values of 1.425 and 1.400 Å. The lengthening of O1—C8 may be attributed to the inductive negative effect of the halogen atom on chroman atom O1. The lengthening of O3—C11 is possibly due to the participation of atom O3 in a relatively strong O—H···N hydrogen bond. In (II), these values are in the range 1.422 (2)–1.4490 (16) Å for O1—C8 and 1.4108 (17)–1.4249 (16) Å for O3—C11.

In both (I) and (II), the chroman system (C1/C2/C7/O1/C8/C9) adopts a screw-boat conformation (Cremer & Pople, 1975), with atoms C8 and O1 deviating from the plane defined by the rest of the atoms. The exception to this is for molecule *A* of (II) where the puckering of the chroman system switches between nearly envelope and screw-boat configurations, owing to the disordered atom O1, which was modelled using two sets of atomic sites with refined occupancies of 0.812 (14) and 0.188 (14). Also, the H atoms on C8*A* are disordered, with refined occupancies of 0.81 (3) and 0.19 (3).The puckering of six-membered rings is measured using three parameters: *Q*, which provides a measure of the magnitude or amplitude of the puckering; θ, which is a descriptor of the type of conformation, *viz.* chair (C), half-chair (H), envelope (E), twist or twist-boat (T), boat (B) or screw-boat (S); and φ, which is an estimate of puckering distortion. θ can take values from 0 to 90°, where 0° represents an ideal chair and 90° an ideal twist conformation; φ ranges from 0 to 360° (Cremer & Pople, 1975). In (II), the puckering of molecules *A*–*F* is described by θ values of 57.6 (4), 63.0 (2), 63.5 (2), 61.8 (2), 67.8 (2) and 64.2 (2)°, respectively. It is seen that molecule *E*, with θ = 67.8 (2)°, conforms closely to the ideal value of 67.5° for a screw-boat conformation.

The hydroxy group and isoxazole ring exhibit an anti-periplanar conformation with respect to atoms O3/C11/C10/

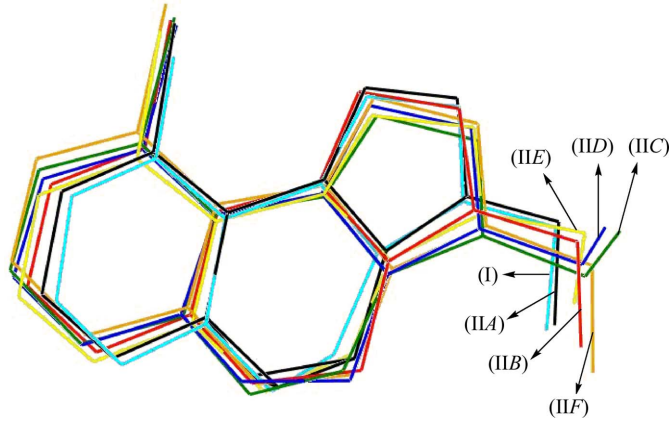

Figure 3
An overlay diagram of (I) and the six molecules in the asymmetric unit of (II). [In the electronic version of the paper, the colour codes are: compound (I) sky blue; compound (II), molecule *A* white, molecule *B* red, molecule *C* green, molecule *D* blue, molecule *E* yellow and molecule *F* orange.]

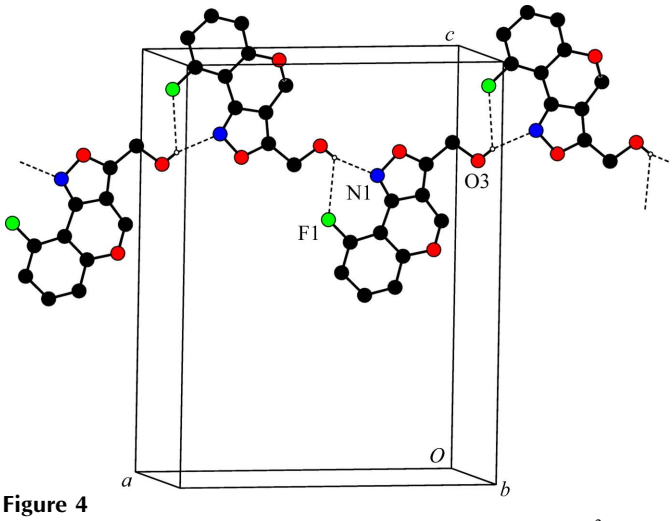

Figure 4
Part of the crystal structure of (I), showing the formation of an $R_1^2(6)$ ring which links the molecules into chains along the *a* axis. Dashed lines indicate hydrogen bonds. For the sake of clarity, H atoms not involved in the ring have been omitted.

O2, defined by an O3—C11—C10—O2 torsion angle of 175.24 (11)° in (I). However, in (II), hydroxy atom O3 has synclinal, synclinal and (−)-antiperiplanar conformations with respect to the isoxazole ring in molecules *C*, *D* and *E*, with values of 76.62 (15), 71.38 (15) and −161.96 (11)°, respectively (Table 3). In molecules *A*, *B* and *F*, hydroxy atom O3 is antiperiplanar with respect to the isoxazole rings, with values of −177.53 (10), 173.12 (11) and 174.06 (11)°, respectively. These differences in conformation may be explained in terms of the mode of participation of atom O3 in the hydrogen-bonding network. Atoms O3 of molecules *C*, *D* and *E* participate as donors in O—H···N and O—H···Cl hydrogen bonds, and as acceptors in O—H···O hydrogen bonds and stronger C—H···O interactions (Table 4). In molecules *A*, *B* and *F*, O—H···N and O—H···Cl hydrogen bonds involving atom O3 are absent. A similar synclinal conformation of −70.23° for the hydroxy O atom has been reported for a

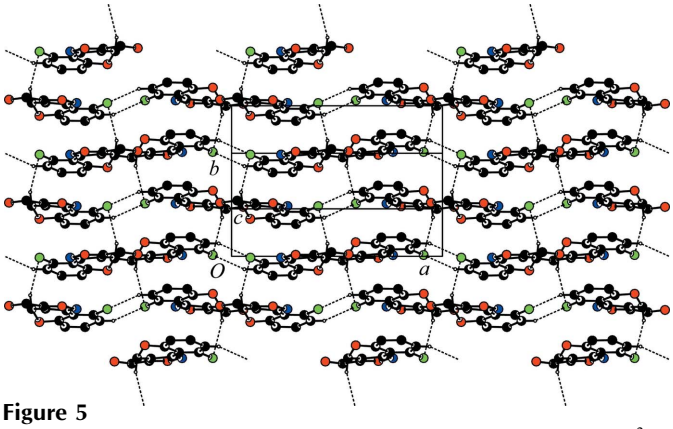

Figure 5
Part of the crystal structure of (I), showing the formation of a cyclic $R_2^2(8)$ motif and a *C*(7) chain *via* C—H···F interactions (dashed lines). For the sake of clarity, H atoms not involved in the motifs shown have been omitted. (In the electronic version of the paper, F atoms are coloured green.)

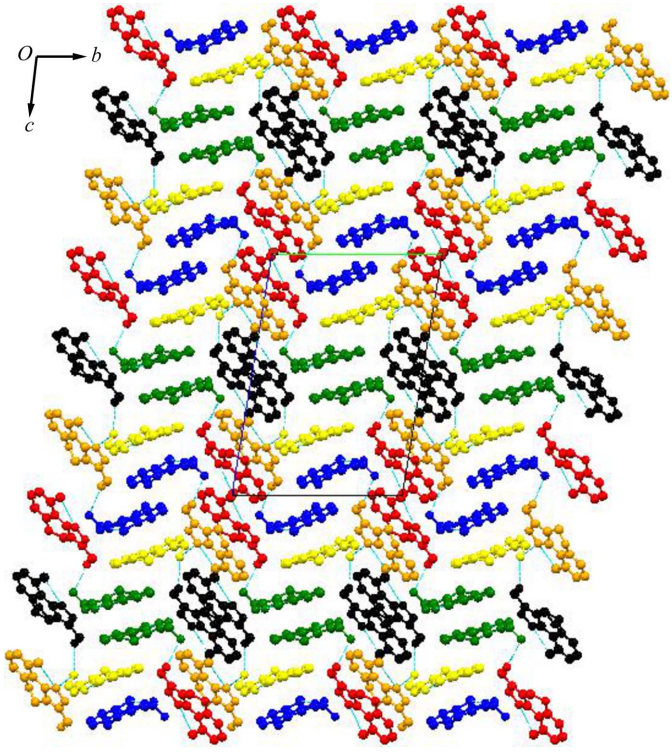

Figure 6
The crystal structure of (II), showing the six molecules in the asymmetric unit. Dashed lines indicate hydrogen bonds. (In the electronic version of the paper, the colour code is: molecule *A* black, molecule *B* red, molecule *C* green, molecule *D* blue, molecule *E* yellow and molecule *F* orange.) Ladder-like arrangements are formed, with the sequence of molecules *C*, *D* and *E* connected between the struts of the ladder sequence of molecules *A*, *B* and *F*.

closely related isoxazoline derivative (Denmark *et al.*, 1999). Fig. 3 shows the superimposition of molecules of (I) and the six molecules of (II), in which the differences in the conformations of the individual molecules can readily be seen.

In (I), the intermolecular interaction pattern is characterized by conventional O—H···N and O—H···F hydrogen-bonded supramolecular motifs. In addition, C—H···F hydrogen bonds between centrosymmetrically related molecules and π–π (arene) interactions combine to generate a two-dimensional hydrogen-bonding network. The overall picture of the intermolecular interactions may be visualized as due to two simple graph-set motifs (Bernstein *et al.*, 1995), *viz.* $R_1^2(6)$ (Fig. 4) and $R_2^2(8)$ (Fig. 5). Firstly, the $R_1^2(6)$ motif is generated through O3—H3···N1^{i} [symmetry code: (i) $x-\frac{1}{2}, y, -z+\frac{3}{2}$] and O3—H3···F1^{i} hydrogen bonds, which link the molecules into one-dimensional chains running parallel to the *a* axis (Fig. 4). These one-dimensional chains have aromatic π–π stacking interactions between the centroids *Cg* and *Cg*($\frac{1}{2}-x, \frac{1}{2}+y, z$) of the fluoro-substituted phenyl rings; the centroid–centroid distance is 3.5925 (7) Å, the interplanar spacing is *ca* 3.51 Å and the ring offset is *ca* 0.76 Å. Secondly, C8—H8*A*···F1($-x+\frac{1}{2}, y-\frac{1}{2}, z$) and C4—H4*A*···F1($-x+1, -y, -z+1$) interactions between centrosymetric pairs form an $R_2^2(8)$ motif. These rings are linked through *C*(7) chains characterized by C—H···F interactions, leading to a two-

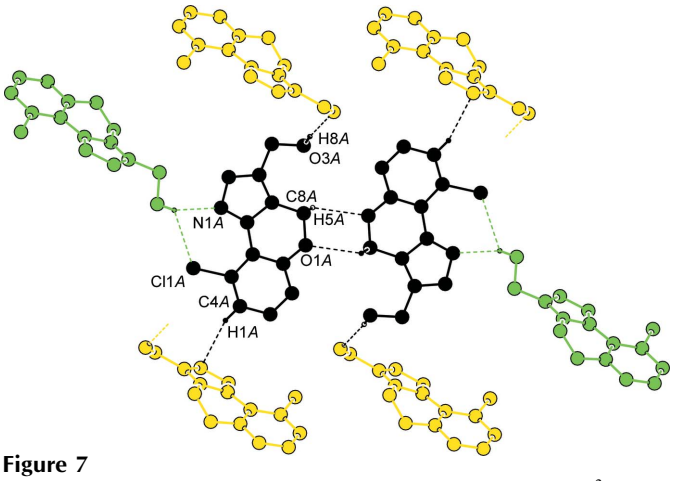

Figure 7
Part of the crystal structure of (II), showing the formation of $R_2^2(6)$ and $R_1^2(6)$ rings involving *A* molecules. Dashed lines indicate hydrogen bonds. For the sake of clarity, H atoms not involved in the motifs have been omitted. (In the electronic version of the paper, the colour code is: molecule *A* black, molecule *C* green and molecule *E* yellow.)

dimensional network. The C—H···F interactions seem to play a proactive role by participating in intermolecular interaction patterns in the absence of conventional hydrogen bonds (Choudhury *et al.*, 2004).

In (II), the geometry of the intermolecular interactions appears complicated due to the presence of six molecules in the asymmetric unit. The interactions are characterized by a combination of conventional O—H···N, O—H···O and O—H···Cl hydrogen bonds. In addition, nonconventional C—H···O, C—H···π and π–π (arene) interactions lead to a three-dimensional hydrogen-bonding network. The complex picture of the intermolecular interaction pattern (Fig. 6) may be simplified in terms of groups of molecules and their roles as donors or acceptors in interactions other than C—H···O. While C—H···O interactions are present involving all six molecules in the asymmetric unit in (II), such commonality is not seen in the cases of the O—H···O, O—H···N and O—H···Cl interactions. In the strong O—H···O hydrogen bonds, atoms O3 of molecules *A*, *B* and *F* participate as donors and those of molecules *C*, *D* and *E* as acceptors. Similarly in the strong O—H···N hydrogen bonds, atoms O3 of molecules *C*, *D* and *E* are donors and atoms N1 of molecules *A*, *B* and *F* are acceptors. Atoms O3 of molecules *C*, *D* and *E* are engaged in O—H ··· Cl interactions, with the Cl atoms of molecules *A*, *B* and *F* as acceptors. The fundamental characteristic motifs are an $R_2^2(6)$ motif generated through the C—H···O hydrogen bonds C8*A*—H8*A*1···O1*A*^{vii} [symmetry code: (vii) $-x+1, -y, -z+1$] (Fig. 7) and C8*D*—H8*D*2···O1*D*^{viii} [symmetry code: (viii) $-x+2, -y+1, -z$] between the chroman systems of centrosymmetric pairs of molecules, an $R_1^2(6)$ motif involving O—H···N and O—H···Cl hydrogen bonds (Fig. 7), an $R_4^4(18)$ motif generated through C4*B*—H4*B*···O2*D*^{v} [symmetry code: (v) $-x+1, -y, -z$] and O3*D*—H30*D*···Cl1*B*^{iii} [symmetry code: (iii) $x+1, y, z$] hydrogen bonds, and an $R_4^4(32)$ motif involving C6*C*—H6*C*···O3*A*^{i} [symmetry code: (i) $-x+1, -y+1, -z+1$] and O3*C*—H30*C*···N1*A*^{iii} hydrogen bonds.

The packing of the six molecules in the asymmetric unit of (II) (Fig. 6) shows a ladder-like arrangement in the groups *ABF* and *CDE* alternate in the sequence *FAAFBBF* and *ECCEDDE*, respectively, as repeat units. The *FAAFBBF* and *ECCEDDE* sequences due to molecules *ABF* (molecular group I) and *CDE* (molecular group II) are further illustrated by the fact that, in group I, the O atom of the hydroxy group is coplanar with the isoxazole ring, with a mean deviation of about 0.2 Å. Such coplanarity is not observed in molecular group II. Furthermore, (I) and molecules *B* and *F* of (II), as well as molecules *A* and *E* of (II), have similar conformations, with slight differences in the O3—C11—C10—O2 torsion angles of the respective molecules (Table 3).

In (I), F···F interactions are absent, which agrees with an earlier observation that the C—F group prefers to form C—H···F interactions rather than F···F contacts and C—H···F interactions prevail over C—H···O interactions (Thalladi *et al.*, 1998). The F1···O1($-x+\frac{1}{2}, y-\frac{1}{2}, z$) [3.1344 (13) Å] interaction gives rise to the interaction of the lone pair of atom O1 with the electron-deficient chroman system, and this type of interaction has also been observed for 6-chloro-2-oxo-2*H*-chromene-3-carboxylate derivatives (Santos-Contreras *et al.*, 2007).

In the crystal packing of (II), three different π–π interactions are observed, with *Cg*···*Cg* distances, interplanar

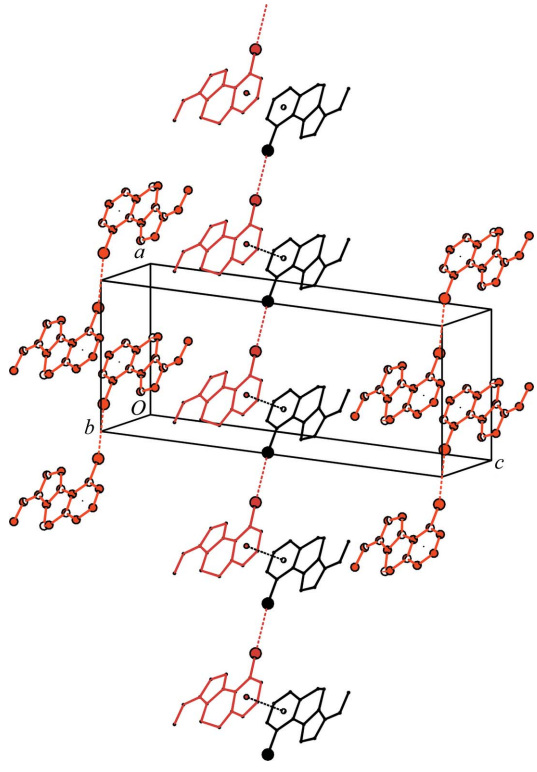

Figure 8
Part of the crystal structure of (II), showing (wireframe atoms) the Cl1*A*···Cl1*F* contacts (dashed lines) between molecules *A* (black) and *F* linked through centroid–centroid interactions between the chloro-substituted benzene rings of the molecules. Also shown (ball-and-stick atoms) are the Cl1*B*···Cl1*B*^{vi} contacts (dashed lines) between molecules *B*. [Symmetry code: (vi) $-x, -y, -z$.]

spacings and ring offsets, respectively, of: (i) 3.5146 (9) Å, *ca* 3.40 Å and *ca* 0.87 Å between the centroids of the chloro-substituted phenyl rings of molecules *A* and *F*($x, y-1, z$); (ii) 3.5783 (8) Å, *ca* 3.21 Å and *ca* 1.58 Å between the isoxazole ring and the chloro-substituted phenyl ring of centrosymmetrically related molecules *C*; and (iii) 3.5597 (8) Å, *ca* 3.29 Å and *ca* 1.35 Å between the isoxazole ring of molecule *D* and the chloro-substituted ring of molecule *E*. A C—H$\cdots\pi$ interaction is also observed between atom H4*A* and the isoxazole ring of molecule *E*, C4*A*—H4*A*$\cdots$*Cg*^{iv} = 2.69 Å and 145° [symmetry code: (iv) $x-1, y-1, z$].

Unlike in (I), hydrogen bonds involving halogens, *i.e.* C—H$\cdots$Cl hydrogen bonds, are absent in (II). However, halogen–halogen interactions, *viz.* two Cl$\cdots$Cl interactions with significant distances are observed in (II), both of type I *trans* geometry (Hathwar *et al.*, 2010; Nayak *et al.*, 2011). The crystal structure of (II) is an example of Cl$\cdots$Cl interactions being preferred as a significant intermolecular constituent in the absence of C—H$\cdots$Cl hydrogen bonds in spite of the larger scope for their presence. In (II), a C3*F*—Cl1*F*$\cdots$Cl1*A*^{v}—C3*A*^{v} interaction is observed between molecules *F* and *A*, with Cl1*F*$\cdots$Cl1*A*^{v} = 3.2105 (4) Å, C3*F*—Cl1*F*$\cdots$Cl1*A*^{v} = 152.02 (5)° and Cl1*F*$\cdots$Cl1*A*^{v}—C3*A*^{v} = 156.54 (5)° [symmetry code: (v) $x+1, y+1, z$] (Fig. 8). There is also a C3*B*—Cl1*B*$\cdots$Cl1*B*^{vi}—C3*B*^{vi} interaction between two molecules *B*, with Cl1*B*$\cdots$Cl1*B*^{vi} = 3.4398 (4) Å and C3*B*—Cl1*B*$\cdots$Cl1*B*^{vi} = 152.22 (5)° [symmetry code: (vi) $-x, -y, -z$] (Fig. 8). It may be inferred that the geometry of both Cl$\cdots$Cl interactions of type I *trans* geometry generates both strong and weak hydrogen bonds and appears to add stability to the crystal packing.

From the above, it may be concluded that the structures of (I) and (II) together demonstrate the subtle nature of the mechanism behind intermolecular interactions and how a simple exchange of substituents may drastically alter the molecular interaction patterns and effect changes in the symmetry of crystal structures. Thus, the structures remain a good example of why crystal structure prediction of small molecules remains a problem as difficult as that of protein folding and, in fact, much more difficult than had been expected.

Experimental

Samples of (I) and (II) were prepared according to the procedure described by Liaskopoulos *et al.* (2007), starting from 2-fluoro- or 2-chloro-6-hydroxybenzaldehyde with 4-chlorobut-2-yn-1-ol in equimolar amounts. Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation from ethanol.

Compound (I)

Crystal data

$C_{11}H_8FNO_3$
M_r = 221.18
Orthorhombic, *Pbca*
a = 14.1516 (2) Å
b = 7.0064 (1) Å
c = 18.3134 (2) Å
V = 1815.81 (4) Å^3
Z = 8
Mo *K*α radiation
μ = 0.13 mm^{-1}
T = 100 K
0.35 × 0.10 × 0.07 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.955, T_{max} = 0.991
18961 measured reflections
3017 independent reflections
2279 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.123
S = 1.05
3017 reflections
149 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °) for (I).

O1—C8	1.4526 (14)	O3—C11	1.4107 (15)
C7—O1—C8—C9	44.47 (14)	O2—C10—C11—O3	175.24 (11)

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O3—H3$\cdots$N1^{i}	0.81 (2)	2.07 (2)	2.8557 (14)	163 (2)
O3—H3$\cdots$F1^{i}	0.81 (2)	2.73 (2)	3.2644 (12)	125.3 (18)
C8—H8*A*$\cdots$F1^{ii}	0.99	2.60	3.5095 (16)	153
C4—H4*A*$\cdots$F1^{iii}	0.95	2.58	3.4674 (14)	155

Symmetry codes: (i) $x-\frac{1}{2}, y, -z+\frac{3}{2}$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, z$; (iii) $-x+1, -y, -z+1$.

Compound (II)

Crystal data

$C_{11}H_8ClNO_3$
M_r = 237.63
Triclinic, $P\overline{1}$
a = 9.4306 (1) Å
b = 14.8892 (2) Å
c = 21.4949 (2) Å
α = 98.764 (1)°
β = 97.610 (1)°
γ = 94.013 (1)°
V = 2944.12 (6) Å^3
Z = 12
Mo *K*α radiation
μ = 0.38 mm^{-1}
T = 100 K
0.32 × 0.32 × 0.17 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.890, T_{max} = 0.937
69911 measured reflections
21416 independent reflections
17626 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
S = 1.04
21416 reflections
900 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

In both compounds, the hydroxy H atoms were located in a difference map and refined freely. All other H atoms were placed geometrically and treated as riding, with C—H = 0.95 (aromatic) or 0.99 Å (methylene) and U_{iso}(H) = 1.2U_{eq}(C). For (II), 17 reflections for which *I*(obs) and *I*(calc) differ more than 10$\sigma(w)$ (the latter being the square root of the weight for that reflection in the least-squares

Table 3
Selected geometric parameters (Å, °) for (II).

Molecule	O1—C8	O3—C11	O2—C10—C11—O3	C7—O1—C8—C9
A	1.422 (2)	1.4136 (17)	−177.53 (10)	34.9 (4)
B	1.4492 (16)	1.4108 (17)	173.12 (11)	40.50 (15)
C	1.4389 (16)	1.4249 (16)	76.62 (15)	−41.90 (16)
D	1.4444 (17)	1.4214 (16)	71.38 (15)	41.39 (16)
E	1.4490 (16)	1.4236 (17)	−161.96 (11)	45.73 (15)
F	1.4463 (16)	1.4121 (18)	174.06 (11)	42.00 (16)

Table 4
Hydrogen-bond geometry (Å, °) for (II).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*A*—H3*OA*···O3*E*^{i}	0.82 (2)	1.99 (2)	2.8006 (14)	165 (2)
O3*B*—H3*OB*···O3*C*	0.82 (2)	1.93 (2)	2.7321 (15)	167 (2)
O3*F*—H3*OF*···O3*D*^{ii}	0.77 (2)	1.99 (2)	2.7535 (15)	170 (2)
O3*C*—H3*OC*···Cl1*A*^{iii}	0.79 (2)	2.73 (2)	3.2601 (11)	126 (2)
O3*D*—H3*OD*···Cl1*B*^{iii}	0.79 (2)	2.83 (2)	3.3070 (11)	120.7 (19)
O3*E*—H3*OE*···Cl1*F*	0.81 (2)	2.89 (2)	3.3580 (11)	118.8 (16)
O3*C*—H3*OC*···N1*A*^{iii}	0.79 (2)	2.10 (2)	2.8471 (15)	158 (2)
O3*D*—H3*OD*···N1*B*^{iii}	0.79 (2)	2.04 (2)	2.8110 (15)	165 (2)
O3*E*—H3*OE*···N1*F*	0.81 (2)	2.04 (2)	2.8132 (15)	160 (2)
C4*A*—H4*A*···O2*E*^{iv}	0.95	2.48	3.3964 (17)	162
C4*B*—H4*B*···O2*D*^{v}	0.95	2.44	3.3457 (16)	160
C4*F*—H4*F*···O2*C*^{vi}	0.95	2.61	3.4190 (17)	144
C8*A*—H8*A*1···O1*A*^{vii}	0.99	2.51	3.122 (3)	120
C8*D*—H8*D*2···O1*D*^{viii}	0.99	2.61	3.3164 (16)	128
C8*F*—H8*F*2···O1*B*^{ix}	0.99	2.60	3.2861 (16)	127
C6*C*—H6*C*···O3*A*^{i}	0.95	2.55	3.4748 (17)	164
C6*E*—H6*E*···O3*B*	0.95	2.36	3.2748 (17)	161
C11*E*—H11*I*···O1*B*^{vi}	0.99	2.53	3.2632 (16)	131

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+1, -z$; (iii) $x+1, y, z$; (iv) $x-1, y-1, z$; (v) $-x+1, -y, -z$; (vi) $x, y+1, z$; (vii) $-x+1, -y, -z+1$; (viii) $-x+2, -y+1, -z$; (ix) $x-1, y+1, z$.

refinement) which are found to be systematic errors have been omitted from the refinement.

For both compounds, data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

The authors thank Dr Mutharasu Devarajan, Associate Professor, and the staff of the X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, for their help in the data collection.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: KU3066). Services for accessing these data are described at the back of the journal.

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supplementary materials

Acta Cryst. (2012). C**68**, o288–o293 [doi:10.1107/S0108270112025620]

Supramolecular networks in (9-fluoro-4*H*-chromeno[4,3-*c*]isoxazol-3-yl)methanol and its 9-chloro analogue at 100 K

P. Rajalakshmi, N. Srinivasan, R. V. Krishnakumar, Ibrahim Abdul Razak and Mohd Mustaqim Rosli

(I) (9-Fluoro-4*H*-chromeno[4,3-*c*]isoxazol-3-yl)methanol

Crystal data

$C_{11}H_8FNO_3$
$M_r = 221.18$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 14.1516$ (2) Å
$b = 7.0064$ (1) Å
$c = 18.3134$ (2) Å
$V = 1815.81$ (4) Å^3
$Z = 8$
$F(000) = 912$
$D_x = 1.618$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3017 reflections
$\theta = 1.0$–$1.0°$
$\mu = 0.13$ mm^{-1}
$T = 100$ K
Block, colourless
0.35 × 0.10 × 0.07 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.955$, $T_{max} = 0.991$
18961 measured reflections
3017 independent reflections
2279 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 31.5°$, $\theta_{min} = 2.2°$
$h = -20 \rightarrow 20$
$k = -10 \rightarrow 10$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.123$
$S = 1.05$
3017 reflections
149 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 0.3939P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.41065 (5)	0.05586 (12)	0.59370 (4)	0.01837 (18)
O1	0.08873 (6)	0.14786 (14)	0.52350 (5)	0.0155 (2)
O2	0.19614 (6)	0.10219 (14)	0.75469 (5)	0.0183 (2)
O3	−0.05528 (7)	0.08591 (17)	0.73037 (5)	0.0249 (2)
N1	0.26517 (7)	0.10383 (17)	0.69879 (6)	0.0169 (2)
C1	0.21639 (8)	0.08882 (17)	0.63780 (6)	0.0127 (2)
C2	0.25101 (8)	0.09622 (18)	0.56288 (6)	0.0123 (2)
C3	0.34492 (8)	0.08806 (18)	0.54103 (6)	0.0134 (2)
C4	0.37431 (9)	0.11263 (19)	0.47017 (7)	0.0158 (2)
H4A	0.4393	0.1052	0.4575	0.019*
C5	0.30535 (9)	0.14883 (19)	0.41753 (7)	0.0169 (3)
H5A	0.3238	0.1702	0.3683	0.020*
C6	0.21028 (9)	0.15418 (19)	0.43580 (6)	0.0159 (2)
H6A	0.1640	0.1759	0.3991	0.019*
C7	0.18288 (8)	0.12752 (18)	0.50808 (6)	0.0132 (2)
C8	0.05216 (8)	0.05084 (19)	0.58765 (6)	0.0148 (2)
H8A	0.0450	−0.0870	0.5772	0.018*
H8B	−0.0108	0.1028	0.6002	0.018*
C9	0.11769 (8)	0.07771 (18)	0.65028 (6)	0.0132 (2)
C10	0.10894 (8)	0.08776 (19)	0.72365 (6)	0.0151 (2)
C11	0.02658 (9)	0.0855 (2)	0.77433 (7)	0.0188 (3)
H11A	0.0282	−0.0301	0.8054	0.023*
H11B	0.0276	0.1994	0.8063	0.023*
H3	−0.0993 (15)	0.095 (3)	0.7581 (12)	0.040 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0095 (3)	0.0282 (5)	0.0175 (3)	0.0019 (3)	−0.0015 (3)	0.0013 (3)
O1	0.0094 (4)	0.0243 (5)	0.0128 (4)	0.0016 (3)	−0.0005 (3)	0.0027 (3)
O2	0.0100 (4)	0.0326 (6)	0.0122 (4)	−0.0010 (3)	0.0004 (3)	0.0006 (4)
O3	0.0099 (4)	0.0485 (7)	0.0161 (4)	0.0013 (4)	0.0013 (3)	0.0009 (4)
N1	0.0102 (4)	0.0277 (6)	0.0128 (4)	−0.0009 (4)	0.0011 (3)	0.0007 (4)
C1	0.0091 (5)	0.0155 (6)	0.0134 (5)	0.0006 (4)	−0.0005 (4)	0.0004 (4)
C2	0.0106 (5)	0.0140 (5)	0.0124 (5)	−0.0001 (4)	0.0000 (4)	0.0005 (4)
C3	0.0094 (5)	0.0155 (6)	0.0155 (5)	0.0002 (4)	−0.0014 (4)	0.0004 (4)
C4	0.0120 (5)	0.0176 (6)	0.0178 (5)	−0.0001 (4)	0.0029 (4)	0.0000 (4)

C5	0.0171 (6)	0.0192 (6)	0.0144 (5)	−0.0002 (5)	0.0030 (4)	0.0008 (4)
C6	0.0157 (5)	0.0186 (6)	0.0134 (5)	0.0010 (5)	0.0000 (4)	0.0007 (4)
C7	0.0108 (5)	0.0153 (6)	0.0136 (5)	0.0008 (4)	−0.0007 (4)	−0.0006 (4)
C8	0.0106 (5)	0.0206 (6)	0.0132 (5)	−0.0010 (4)	0.0000 (4)	0.0016 (4)
C9	0.0089 (5)	0.0174 (6)	0.0134 (5)	0.0002 (4)	−0.0005 (4)	0.0010 (4)
C10	0.0094 (5)	0.0215 (6)	0.0146 (5)	0.0006 (4)	−0.0005 (4)	0.0002 (5)
C11	0.0117 (5)	0.0307 (8)	0.0141 (5)	0.0009 (5)	0.0023 (4)	0.0006 (5)

Geometric parameters (Å, º)

F1—C3	1.3589 (13)	C4—C5	1.3949 (17)
O1—C7	1.3693 (13)	C4—H4A	0.9500
O1—C8	1.4526 (14)	C5—C6	1.3870 (17)
O2—C10	1.3624 (14)	C5—H5A	0.9500
O2—N1	1.4151 (13)	C6—C7	1.3919 (16)
O3—C11	1.4107 (15)	C6—H6A	0.9500
O3—H3	0.81 (2)	C8—C9	1.4870 (16)
N1—C1	1.3172 (15)	C8—H8A	0.9900
C1—C9	1.4175 (16)	C8—H8B	0.9900
C1—C2	1.4577 (16)	C9—C10	1.3512 (16)
C2—C3	1.3891 (16)	C10—C11	1.4901 (17)
C2—C7	1.4089 (16)	C11—H11A	0.9900
C3—C4	1.3736 (16)	C11—H11B	0.9900
C7—O1—C8	117.70 (9)	O1—C7—C6	116.95 (10)
C10—O2—N1	108.91 (9)	O1—C7—C2	122.36 (10)
C11—O3—H3	105.9 (15)	C6—C7—C2	120.51 (11)
C1—N1—O2	104.54 (9)	O1—C8—C9	110.02 (9)
N1—C1—C9	112.59 (10)	O1—C8—H8A	109.7
N1—C1—C2	128.25 (11)	C9—C8—H8A	109.7
C9—C1—C2	119.01 (10)	O1—C8—H8B	109.7
C3—C2—C7	117.13 (10)	C9—C8—H8B	109.7
C3—C2—C1	126.25 (11)	H8A—C8—H8B	108.2
C7—C2—C1	116.48 (10)	C10—C9—C1	104.35 (10)
F1—C3—C4	118.96 (10)	C10—C9—C8	135.76 (11)
F1—C3—C2	117.21 (10)	C1—C9—C8	119.81 (10)
C4—C3—C2	123.83 (11)	C9—C10—O2	109.61 (10)
C3—C4—C5	117.64 (11)	C9—C10—C11	133.68 (11)
C3—C4—H4A	121.2	O2—C10—C11	116.70 (10)
C5—C4—H4A	121.2	O3—C11—C10	106.66 (10)
C6—C5—C4	121.12 (11)	O3—C11—H11A	110.4
C6—C5—H5A	119.4	C10—C11—H11A	110.4
C4—C5—H5A	119.4	O3—C11—H11B	110.4
C5—C6—C7	119.74 (11)	C10—C11—H11B	110.4
C5—C6—H6A	120.1	H11A—C11—H11B	108.6
C7—C6—H6A	120.1		
C10—O2—N1—C1	−0.52 (13)	C3—C2—C7—O1	−176.63 (11)
O2—N1—C1—C9	0.16 (14)	C1—C2—C7—O1	−0.77 (18)
O2—N1—C1—C2	175.44 (12)	C3—C2—C7—C6	−1.77 (18)

N1—C1—C2—C3	11.9 (2)	C1—C2—C7—C6	174.09 (12)
C9—C1—C2—C3	−173.10 (12)	C7—O1—C8—C9	44.47 (14)
N1—C1—C2—C7	−163.55 (13)	N1—C1—C9—C10	0.24 (15)
C9—C1—C2—C7	11.46 (17)	C2—C1—C9—C10	−175.52 (11)
C7—C2—C3—F1	−179.32 (11)	N1—C1—C9—C8	−177.07 (11)
C1—C2—C3—F1	5.27 (19)	C2—C1—C9—C8	7.17 (17)
C7—C2—C3—C4	1.43 (19)	O1—C8—C9—C10	149.93 (15)
C1—C2—C3—C4	−173.97 (12)	O1—C8—C9—C1	−33.80 (16)
F1—C3—C4—C5	−178.88 (11)	C1—C9—C10—O2	−0.57 (14)
C2—C3—C4—C5	0.35 (19)	C8—C9—C10—O2	176.10 (13)
C3—C4—C5—C6	−1.86 (19)	C1—C9—C10—C11	179.68 (14)
C4—C5—C6—C7	1.5 (2)	C8—C9—C10—C11	−3.7 (3)
C8—O1—C7—C6	155.91 (11)	N1—O2—C10—C9	0.69 (14)
C8—O1—C7—C2	−29.06 (17)	N1—O2—C10—C11	−179.51 (11)
C5—C6—C7—O1	175.49 (12)	C9—C10—C11—O3	−5.0 (2)
C5—C6—C7—C2	0.36 (19)	O2—C10—C11—O3	175.24 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···N1^{i}	0.81 (2)	2.07 (2)	2.8557 (14)	163 (2)
O3—H3···F1^{i}	0.81 (2)	2.73 (2)	3.2644 (12)	125.3 (18)
C8—H8*A*···F1^{ii}	0.99	2.60	3.5095 (16)	153
C4—H4*A*···F1^{iii}	0.95	2.58	3.4674 (14)	155

Symmetry codes: (i) *x*−1/2, *y*, −*z*+3/2; (ii) −*x*+1/2, *y*−1/2, *z*; (iii) −*x*+1, −*y*, −*z*+1.

(II) (9-Chloro-4*H*-chromeno[4,3-*c*]isoxazol-3-yl)methanol

Crystal data

$C_{11}H_8ClNO_3$
M_r = 237.63
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.4306 (1) Å
b = 14.8892 (2) Å
c = 21.4949 (2) Å
α = 98.764 (1)°
β = 97.610 (1)°
γ = 94.013 (1)°
V = 2944.12 (6) Å^3
Z = 12
F(000) = 1464
D_x = 1.608 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 17629 reflections
θ = 2–32.7°
μ = 0.38 mm^{-1}
T = 100 K
Block, colourless
0.32 × 0.32 × 0.17 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.890, T_{max} = 0.937
69911 measured reflections
21416 independent reflections
17626 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 32.7°, θ_{min} = 1.0°
h = −14→11
k = −22→22
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.107$
$S = 1.04$
21416 reflections
900 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 1.7339P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.66$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1A	−0.14998 (3)	−0.02223 (2)	0.341046 (16)	0.01868 (7)	
O1A	0.3263 (3)	−0.04319 (16)	0.48527 (17)	0.0180 (6)	0.812 (14)
O1X	0.3545 (9)	−0.0222 (8)	0.4646 (6)	0.015 (3)	0.188 (14)
O2A	0.03088 (10)	0.18351 (6)	0.50824 (4)	0.01526 (17)	
O3A	0.36968 (11)	0.22168 (7)	0.61306 (5)	0.0195 (2)	
H3OA	0.379 (2)	0.2259 (15)	0.6521 (11)	0.044 (6)*	
N1A	−0.01383 (12)	0.11003 (7)	0.45750 (5)	0.0156 (2)	
C1A	0.09396 (13)	0.05807 (8)	0.45789 (6)	0.0122 (2)	
C2A	0.10778 (13)	−0.02564 (8)	0.41479 (6)	0.0125 (2)	
C3A	0.01191 (14)	−0.06649 (9)	0.36080 (6)	0.0141 (2)	
C4A	0.04135 (15)	−0.14352 (9)	0.32123 (6)	0.0172 (2)	
H4A	−0.0251	−0.1694	0.2847	0.021*	
C5A	0.16873 (15)	−0.18245 (9)	0.33552 (7)	0.0185 (3)	
H5A	0.1900	−0.2347	0.3083	0.022*	
C6A	0.26491 (15)	−0.14568 (9)	0.38919 (7)	0.0194 (3)	
H6A	0.3514	−0.1730	0.3991	0.023*	
C7A	0.23422 (14)	−0.06836 (9)	0.42877 (7)	0.0169 (2)	
C8A	0.34386 (15)	0.04933 (10)	0.51591 (7)	0.0205 (3)	
H8A1	0.4188	0.0833	0.4982	0.025*	0.81 (3)
H8A2	0.3767	0.0519	0.5619	0.025*	0.81 (3)
H8X1	0.4259	0.0961	0.5197	0.025*	0.19 (3)
H8X2	0.3509	0.0240	0.5561	0.025*	0.19 (3)
C9A	0.20827 (13)	0.09350 (8)	0.50748 (6)	0.0126 (2)	
C10A	0.16384 (13)	0.17117 (8)	0.53679 (6)	0.0129 (2)	
C11A	0.23024 (14)	0.24317 (9)	0.59090 (6)	0.0159 (2)	

H11A	0.2357	0.3033	0.5767	0.019*
H11B	0.1707	0.2463	0.6257	0.019*
Cl1B	0.18312 (3)	−0.00439 (2)	0.007443 (15)	0.01776 (6)
O1B	0.65963 (10)	−0.04228 (6)	0.14643 (5)	0.01632 (18)
O2B	0.36463 (10)	0.18042 (6)	0.18437 (4)	0.01489 (17)
O3B	0.70827 (11)	0.21754 (7)	0.28708 (5)	0.0205 (2)
H3OB	0.701 (2)	0.1947 (15)	0.3188 (11)	0.045 (7)*
N1B	0.31605 (12)	0.10962 (7)	0.13235 (5)	0.0146 (2)
C1B	0.42644 (13)	0.06067 (8)	0.12689 (6)	0.0117 (2)
C2B	0.43645 (13)	−0.02100 (8)	0.08103 (6)	0.0124 (2)
C3B	0.33814 (14)	−0.05676 (9)	0.02649 (6)	0.0140 (2)
C4B	0.36119 (15)	−0.13382 (9)	−0.01452 (6)	0.0175 (2)
H4B	0.2927	−0.1570	−0.0510	0.021*
C5B	0.48529 (16)	−0.17698 (9)	−0.00192 (7)	0.0185 (3)
H5B	0.5022	−0.2292	−0.0303	0.022*
C6B	0.58482 (15)	−0.14450 (9)	0.05179 (7)	0.0175 (2)
H6B	0.6691	−0.1746	0.0604	0.021*
C7B	0.55993 (14)	−0.06715 (8)	0.09308 (6)	0.0135 (2)
C8B	0.68482 (14)	0.05323 (9)	0.17478 (6)	0.0151 (2)
H8B1	0.7491	0.0856	0.1509	0.018*
H8B2	0.7326	0.0589	0.2193	0.018*
C9B	0.54673 (13)	0.09544 (8)	0.17372 (6)	0.0126 (2)
C10B	0.50235 (13)	0.16982 (8)	0.20769 (6)	0.0133 (2)
C11B	0.57240 (15)	0.24080 (9)	0.26190 (6)	0.0168 (2)
H11C	0.5837	0.3003	0.2471	0.020*
H11D	0.5102	0.2472	0.2957	0.020*
Cl1C	0.09523 (4)	0.37951 (2)	0.455536 (18)	0.02131 (7)
O1C	0.58055 (10)	0.52058 (6)	0.41069 (5)	0.01714 (18)
O2C	0.49604 (10)	0.24970 (6)	0.47468 (5)	0.01595 (18)
O3C	0.71868 (12)	0.16202 (7)	0.40291 (5)	0.0190 (2)
H3OC	0.787 (2)	0.1352 (15)	0.4106 (11)	0.041 (6)*
N1C	0.37986 (12)	0.30420 (7)	0.47093 (5)	0.0151 (2)
C1C	0.42434 (14)	0.37225 (8)	0.44320 (6)	0.0131 (2)
C2C	0.35011 (14)	0.45159 (8)	0.42988 (6)	0.0130 (2)
C3C	0.20640 (14)	0.46471 (9)	0.43480 (6)	0.0152 (2)
C4C	0.14740 (15)	0.54412 (9)	0.42267 (7)	0.0186 (3)
H4C	0.0494	0.5516	0.4262	0.022*
C5C	0.23469 (16)	0.61264 (9)	0.40524 (7)	0.0191 (3)
H5C	0.1951	0.6672	0.3967	0.023*
C6C	0.37812 (16)	0.60314 (9)	0.40009 (6)	0.0170 (2)
H6C	0.4363	0.6507	0.3884	0.020*
C7C	0.43554 (14)	0.52288 (9)	0.41238 (6)	0.0145 (2)
C8C	0.63505 (15)	0.43324 (9)	0.39545 (7)	0.0185 (3)
H8C1	0.7404	0.4391	0.4086	0.022*
H8C2	0.6156	0.4125	0.3489	0.022*
C9C	0.56617 (14)	0.36461 (9)	0.42847 (6)	0.0139 (2)
C10C	0.60563 (14)	0.28788 (9)	0.44945 (6)	0.0151 (2)
C11C	0.73922 (15)	0.24061 (9)	0.45123 (7)	0.0183 (2)
H11E	0.8198	0.2824	0.4443	0.022*

H11F	0.7635	0.2222	0.4934	0.022*
Cl1D	0.43836 (4)	0.39893 (2)	0.147509 (19)	0.02281 (7)
O1D	0.87174 (11)	0.50326 (7)	0.04379 (5)	0.0215 (2)
O2D	0.83028 (10)	0.25964 (6)	0.14473 (5)	0.01633 (18)
O3D	1.06485 (12)	0.18025 (7)	0.08209 (5)	0.0193 (2)
H3OD	1.133 (2)	0.1533 (15)	0.0903 (11)	0.042 (6)*
N1D	0.70895 (12)	0.30949 (7)	0.13738 (5)	0.0150 (2)
C1D	0.75425 (13)	0.38151 (8)	0.11399 (6)	0.0128 (2)
C2D	0.67267 (14)	0.45686 (8)	0.09742 (6)	0.0135 (2)
C3D	0.53465 (14)	0.47392 (9)	0.11069 (6)	0.0161 (2)
C4D	0.46861 (16)	0.54864 (10)	0.09360 (7)	0.0205 (3)
H4D	0.3748	0.5588	0.1029	0.025*
C5D	0.54207 (17)	0.60843 (10)	0.06259 (7)	0.0223 (3)
H5D	0.4979	0.6601	0.0510	0.027*
C6D	0.67863 (17)	0.59400 (10)	0.04824 (7)	0.0211 (3)
H6D	0.7277	0.6355	0.0272	0.025*
C7D	0.74285 (15)	0.51833 (9)	0.06497 (6)	0.0169 (2)
C8D	0.97477 (15)	0.45798 (10)	0.08094 (7)	0.0183 (2)
H8D1	1.0261	0.5022	0.1174	0.022*
H8D2	1.0464	0.4344	0.0544	0.022*
C9D	0.90095 (14)	0.38096 (9)	0.10479 (6)	0.0144 (2)
C10D	0.94288 (14)	0.30379 (9)	0.12469 (6)	0.0155 (2)
C11D	1.07974 (15)	0.25993 (10)	0.12906 (7)	0.0197 (3)
H11G	1.1589	0.3029	0.1222	0.024*
H11H	1.1032	0.2434	0.1719	0.024*
Cl1E	1.25397 (4)	0.59857 (2)	0.228807 (17)	0.01890 (7)
O1E	0.74285 (10)	0.48379 (6)	0.26095 (5)	0.01528 (17)
O2E	0.86544 (10)	0.73553 (6)	0.18238 (5)	0.01656 (18)
O3E	0.54653 (11)	0.75356 (7)	0.25506 (5)	0.01846 (19)
H3OE	0.480 (2)	0.7836 (14)	0.2481 (10)	0.030 (5)*
N1E	0.97307 (13)	0.67528 (8)	0.19125 (6)	0.0162 (2)
C1E	0.91909 (14)	0.61778 (8)	0.22482 (6)	0.0131 (2)
C2E	0.98418 (14)	0.53930 (8)	0.24620 (6)	0.0128 (2)
C3E	1.12800 (14)	0.52064 (9)	0.24838 (6)	0.0145 (2)
C4E	1.17572 (15)	0.44091 (9)	0.26623 (6)	0.0168 (2)
H4E	1.2738	0.4295	0.2672	0.020*
C5E	1.07635 (16)	0.37797 (9)	0.28267 (6)	0.0183 (3)
H5E	1.1079	0.3230	0.2946	0.022*
C6E	0.93318 (15)	0.39328 (9)	0.28216 (6)	0.0153 (2)
H6E	0.8673	0.3497	0.2937	0.018*
C7E	0.88751 (14)	0.47437 (8)	0.26431 (6)	0.0136 (2)
C8E	0.69849 (15)	0.57529 (9)	0.27309 (6)	0.0162 (2)
H8E1	0.7184	0.5992	0.3193	0.019*
H8E2	0.5939	0.5742	0.2592	0.019*
C9E	0.77880 (14)	0.63571 (8)	0.23763 (6)	0.0133 (2)
C10E	0.75162 (14)	0.71038 (9)	0.21058 (6)	0.0145 (2)
C11E	0.63294 (15)	0.77103 (10)	0.20794 (7)	0.0183 (2)
H11I	0.6726	0.8358	0.2163	0.022*
H11J	0.5745	0.7585	0.1653	0.022*

Cl1F	0.50816 (3)	0.97439 (2)	0.304531 (16)	0.01865 (7)
O1F	−0.00859 (10)	1.00507 (7)	0.20275 (5)	0.01909 (19)
O2F	0.26715 (10)	0.77997 (6)	0.14538 (5)	0.01671 (18)
O3F	−0.06379 (12)	0.77588 (8)	0.03786 (5)	0.0230 (2)
H3OF	−0.058 (2)	0.7931 (15)	0.0061 (11)	0.040 (6)*
N1F	0.32382 (12)	0.84505 (8)	0.19971 (5)	0.0155 (2)
C1F	0.23417 (13)	0.90927 (9)	0.20075 (6)	0.0127 (2)
C2F	0.23864 (13)	0.99192 (8)	0.24764 (6)	0.0127 (2)
C3F	0.35112 (14)	1.02804 (9)	0.29641 (6)	0.0147 (2)
C4F	0.34082 (15)	1.10536 (9)	0.33993 (6)	0.0174 (2)
H4F	0.4186	1.1282	0.3726	0.021*
C5F	0.21503 (15)	1.14915 (9)	0.33524 (7)	0.0182 (2)
H5F	0.2069	1.2020	0.3650	0.022*
C6F	0.10138 (15)	1.11628 (9)	0.28742 (7)	0.0174 (2)
H6F	0.0163	1.1469	0.2841	0.021*
C7F	0.11265 (14)	1.03824 (9)	0.24435 (6)	0.0144 (2)
C8F	0.00595 (14)	0.95296 (9)	0.14176 (6)	0.0168 (2)
H8F1	0.0319	0.9949	0.1127	0.020*
H8F2	−0.0869	0.9181	0.1227	0.020*
C9F	0.11870 (13)	0.88901 (9)	0.14956 (6)	0.0128 (2)
C10F	0.14468 (14)	0.80791 (9)	0.11709 (6)	0.0147 (2)
C11F	0.06913 (15)	0.74491 (10)	0.05961 (6)	0.0187 (3)
H11K	0.1303	0.7412	0.0254	0.022*
H11L	0.0526	0.6830	0.0702	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1A	0.01398 (14)	0.02265 (15)	0.01694 (14)	0.00393 (11)	−0.00300 (11)	−0.00105 (11)
O1A	0.0146 (7)	0.0152 (7)	0.0227 (11)	0.0045 (6)	−0.0027 (7)	0.0016 (7)
O1X	0.011 (3)	0.017 (3)	0.015 (4)	0.003 (2)	−0.001 (2)	−0.002 (3)
O2A	0.0139 (4)	0.0142 (4)	0.0160 (4)	0.0039 (3)	−0.0012 (3)	−0.0014 (3)
O3A	0.0148 (5)	0.0270 (5)	0.0147 (5)	0.0010 (4)	−0.0016 (4)	0.0009 (4)
N1A	0.0147 (5)	0.0128 (5)	0.0169 (5)	0.0027 (4)	−0.0018 (4)	−0.0021 (4)
C1A	0.0115 (5)	0.0122 (5)	0.0135 (5)	0.0018 (4)	0.0020 (4)	0.0031 (4)
C2A	0.0113 (5)	0.0121 (5)	0.0144 (5)	0.0008 (4)	0.0020 (4)	0.0032 (4)
C3A	0.0151 (6)	0.0145 (5)	0.0129 (5)	0.0020 (4)	0.0024 (4)	0.0029 (4)
C4A	0.0205 (6)	0.0155 (6)	0.0148 (6)	0.0001 (5)	0.0025 (5)	0.0011 (4)
C5A	0.0227 (7)	0.0128 (5)	0.0213 (6)	0.0016 (5)	0.0087 (5)	0.0021 (5)
C6A	0.0172 (6)	0.0142 (6)	0.0268 (7)	0.0040 (5)	0.0046 (5)	0.0010 (5)
C7A	0.0131 (6)	0.0147 (5)	0.0217 (6)	0.0025 (4)	0.0002 (5)	0.0001 (5)
C8A	0.0163 (6)	0.0206 (6)	0.0214 (6)	0.0072 (5)	−0.0036 (5)	−0.0035 (5)
C9A	0.0110 (5)	0.0139 (5)	0.0128 (5)	0.0007 (4)	0.0002 (4)	0.0032 (4)
C10A	0.0115 (5)	0.0142 (5)	0.0128 (5)	0.0006 (4)	0.0003 (4)	0.0034 (4)
C11A	0.0163 (6)	0.0157 (5)	0.0143 (5)	−0.0004 (5)	0.0013 (4)	−0.0001 (4)
Cl1B	0.01400 (14)	0.02275 (15)	0.01492 (13)	0.00193 (11)	−0.00224 (10)	0.00164 (11)
O1B	0.0149 (4)	0.0133 (4)	0.0194 (5)	0.0030 (3)	−0.0027 (3)	0.0020 (3)
O2B	0.0144 (4)	0.0147 (4)	0.0142 (4)	0.0037 (3)	−0.0006 (3)	−0.0007 (3)
O3B	0.0179 (5)	0.0242 (5)	0.0177 (5)	−0.0032 (4)	−0.0035 (4)	0.0061 (4)
N1B	0.0137 (5)	0.0146 (5)	0.0139 (5)	0.0020 (4)	−0.0008 (4)	−0.0007 (4)

C1B	0.0108 (5)	0.0124 (5)	0.0120 (5)	0.0013 (4)	0.0009 (4)	0.0032 (4)
C2B	0.0117 (5)	0.0126 (5)	0.0130 (5)	0.0004 (4)	0.0021 (4)	0.0029 (4)
C3B	0.0134 (5)	0.0157 (5)	0.0128 (5)	0.0002 (4)	0.0010 (4)	0.0035 (4)
C4B	0.0220 (6)	0.0156 (6)	0.0136 (6)	−0.0024 (5)	0.0021 (5)	0.0007 (4)
C5B	0.0248 (7)	0.0122 (5)	0.0189 (6)	0.0011 (5)	0.0064 (5)	0.0010 (5)
C6B	0.0198 (6)	0.0137 (5)	0.0207 (6)	0.0042 (5)	0.0059 (5)	0.0041 (5)
C7B	0.0128 (5)	0.0132 (5)	0.0149 (5)	0.0010 (4)	0.0024 (4)	0.0031 (4)
C8B	0.0119 (5)	0.0149 (5)	0.0177 (6)	0.0019 (4)	−0.0001 (4)	0.0019 (4)
C9B	0.0115 (5)	0.0135 (5)	0.0130 (5)	0.0017 (4)	0.0004 (4)	0.0035 (4)
C10B	0.0126 (5)	0.0138 (5)	0.0133 (5)	0.0017 (4)	−0.0002 (4)	0.0031 (4)
C11B	0.0196 (6)	0.0153 (6)	0.0140 (5)	−0.0005 (5)	−0.0001 (5)	0.0009 (4)
Cl1C	0.01531 (14)	0.02242 (15)	0.02859 (17)	0.00173 (12)	0.00697 (12)	0.00844 (13)
O1C	0.0165 (4)	0.0137 (4)	0.0216 (5)	−0.0001 (3)	0.0052 (4)	0.0027 (3)
O2C	0.0168 (4)	0.0135 (4)	0.0184 (4)	0.0038 (3)	0.0029 (4)	0.0038 (3)
O3C	0.0207 (5)	0.0182 (5)	0.0173 (5)	0.0094 (4)	−0.0013 (4)	0.0002 (4)
N1C	0.0149 (5)	0.0129 (5)	0.0183 (5)	0.0028 (4)	0.0038 (4)	0.0033 (4)
C1C	0.0141 (5)	0.0128 (5)	0.0119 (5)	0.0008 (4)	0.0018 (4)	0.0012 (4)
C2C	0.0150 (6)	0.0119 (5)	0.0122 (5)	0.0016 (4)	0.0021 (4)	0.0017 (4)
C3C	0.0151 (6)	0.0160 (5)	0.0145 (5)	0.0013 (4)	0.0029 (4)	0.0018 (4)
C4C	0.0190 (6)	0.0192 (6)	0.0174 (6)	0.0058 (5)	0.0013 (5)	0.0015 (5)
C5C	0.0264 (7)	0.0140 (6)	0.0162 (6)	0.0057 (5)	−0.0004 (5)	0.0012 (5)
C6C	0.0240 (7)	0.0118 (5)	0.0143 (6)	0.0021 (5)	−0.0002 (5)	0.0015 (4)
C7C	0.0173 (6)	0.0135 (5)	0.0120 (5)	0.0001 (4)	0.0012 (4)	0.0012 (4)
C8C	0.0191 (6)	0.0166 (6)	0.0213 (6)	0.0010 (5)	0.0083 (5)	0.0033 (5)
C9C	0.0137 (5)	0.0146 (5)	0.0132 (5)	0.0008 (4)	0.0026 (4)	0.0013 (4)
C10C	0.0153 (6)	0.0147 (5)	0.0141 (5)	0.0019 (4)	0.0006 (4)	−0.0001 (4)
C11C	0.0157 (6)	0.0168 (6)	0.0209 (6)	0.0044 (5)	0.0002 (5)	−0.0004 (5)
Cl1D	0.01586 (15)	0.02262 (16)	0.03299 (19)	0.00284 (12)	0.00784 (13)	0.00992 (14)
O1D	0.0224 (5)	0.0256 (5)	0.0205 (5)	0.0051 (4)	0.0084 (4)	0.0106 (4)
O2D	0.0159 (4)	0.0137 (4)	0.0195 (5)	0.0034 (3)	0.0016 (4)	0.0027 (3)
O3D	0.0210 (5)	0.0186 (5)	0.0163 (4)	0.0092 (4)	−0.0023 (4)	−0.0022 (4)
N1D	0.0141 (5)	0.0136 (5)	0.0176 (5)	0.0028 (4)	0.0025 (4)	0.0022 (4)
C1D	0.0130 (5)	0.0131 (5)	0.0117 (5)	0.0010 (4)	0.0016 (4)	0.0008 (4)
C2D	0.0143 (5)	0.0126 (5)	0.0131 (5)	0.0014 (4)	0.0006 (4)	0.0012 (4)
C3D	0.0163 (6)	0.0153 (5)	0.0162 (6)	0.0007 (5)	0.0013 (5)	0.0021 (4)
C4D	0.0197 (6)	0.0192 (6)	0.0225 (7)	0.0060 (5)	0.0017 (5)	0.0023 (5)
C5D	0.0280 (7)	0.0172 (6)	0.0217 (7)	0.0064 (5)	−0.0008 (6)	0.0046 (5)
C6D	0.0274 (7)	0.0176 (6)	0.0191 (6)	0.0023 (5)	0.0025 (5)	0.0060 (5)
C7D	0.0201 (6)	0.0166 (6)	0.0142 (6)	0.0014 (5)	0.0027 (5)	0.0029 (4)
C8D	0.0168 (6)	0.0209 (6)	0.0182 (6)	0.0006 (5)	0.0051 (5)	0.0047 (5)
C9D	0.0145 (6)	0.0161 (5)	0.0119 (5)	0.0011 (4)	0.0020 (4)	0.0006 (4)
C10D	0.0137 (6)	0.0158 (5)	0.0154 (6)	0.0024 (4)	0.0005 (4)	−0.0016 (4)
C11D	0.0163 (6)	0.0192 (6)	0.0206 (6)	0.0041 (5)	−0.0022 (5)	−0.0028 (5)
Cl1E	0.01560 (14)	0.01716 (14)	0.02477 (16)	0.00139 (11)	0.00683 (12)	0.00269 (12)
O1E	0.0145 (4)	0.0123 (4)	0.0194 (4)	0.0011 (3)	0.0033 (3)	0.0030 (3)
O2E	0.0179 (5)	0.0157 (4)	0.0183 (4)	0.0045 (4)	0.0047 (4)	0.0069 (3)
O3E	0.0167 (5)	0.0233 (5)	0.0176 (5)	0.0085 (4)	0.0030 (4)	0.0068 (4)
N1E	0.0177 (5)	0.0146 (5)	0.0179 (5)	0.0037 (4)	0.0045 (4)	0.0048 (4)
C1E	0.0152 (6)	0.0119 (5)	0.0120 (5)	0.0020 (4)	0.0020 (4)	0.0006 (4)

C2E	0.0147 (5)	0.0107 (5)	0.0126 (5)	0.0018 (4)	0.0017 (4)	0.0009 (4)
C3E	0.0153 (6)	0.0135 (5)	0.0140 (5)	0.0013 (4)	0.0028 (4)	−0.0002 (4)
C4E	0.0173 (6)	0.0161 (6)	0.0163 (6)	0.0050 (5)	0.0008 (5)	0.0006 (5)
C5E	0.0245 (7)	0.0134 (5)	0.0166 (6)	0.0044 (5)	0.0002 (5)	0.0017 (5)
C6E	0.0197 (6)	0.0121 (5)	0.0133 (5)	0.0014 (5)	0.0007 (5)	0.0012 (4)
C7E	0.0158 (6)	0.0129 (5)	0.0114 (5)	0.0017 (4)	0.0011 (4)	0.0007 (4)
C8E	0.0175 (6)	0.0141 (5)	0.0185 (6)	0.0022 (5)	0.0062 (5)	0.0035 (5)
C9E	0.0146 (5)	0.0124 (5)	0.0129 (5)	0.0018 (4)	0.0023 (4)	0.0015 (4)
C10E	0.0148 (6)	0.0146 (5)	0.0138 (5)	0.0006 (4)	0.0019 (4)	0.0020 (4)
C11E	0.0210 (6)	0.0197 (6)	0.0167 (6)	0.0074 (5)	0.0038 (5)	0.0066 (5)
Cl1F	0.01254 (13)	0.02157 (15)	0.02018 (15)	0.00260 (11)	−0.00279 (11)	0.00216 (12)
O1F	0.0127 (4)	0.0250 (5)	0.0177 (5)	0.0059 (4)	−0.0012 (3)	−0.0013 (4)
O2F	0.0173 (4)	0.0171 (4)	0.0146 (4)	0.0048 (4)	−0.0004 (3)	0.0000 (3)
O3F	0.0182 (5)	0.0333 (6)	0.0167 (5)	0.0006 (4)	−0.0020 (4)	0.0062 (4)
N1F	0.0149 (5)	0.0172 (5)	0.0137 (5)	0.0048 (4)	−0.0002 (4)	0.0003 (4)
C1F	0.0095 (5)	0.0161 (5)	0.0133 (5)	0.0014 (4)	0.0018 (4)	0.0046 (4)
C2F	0.0105 (5)	0.0143 (5)	0.0142 (5)	0.0012 (4)	0.0017 (4)	0.0049 (4)
C3F	0.0125 (5)	0.0166 (6)	0.0154 (6)	0.0011 (4)	0.0013 (4)	0.0051 (4)
C4F	0.0188 (6)	0.0166 (6)	0.0157 (6)	−0.0019 (5)	0.0012 (5)	0.0022 (5)
C5F	0.0231 (7)	0.0135 (5)	0.0185 (6)	0.0015 (5)	0.0057 (5)	0.0019 (5)
C6F	0.0182 (6)	0.0154 (6)	0.0200 (6)	0.0048 (5)	0.0049 (5)	0.0041 (5)
C7F	0.0123 (5)	0.0161 (5)	0.0151 (5)	0.0027 (4)	0.0011 (4)	0.0039 (4)
C8F	0.0136 (6)	0.0213 (6)	0.0153 (6)	0.0054 (5)	−0.0004 (4)	0.0025 (5)
C9F	0.0098 (5)	0.0157 (5)	0.0133 (5)	0.0010 (4)	0.0012 (4)	0.0048 (4)
C10F	0.0138 (5)	0.0181 (6)	0.0127 (5)	0.0017 (4)	0.0017 (4)	0.0046 (4)
C11F	0.0198 (6)	0.0202 (6)	0.0148 (6)	0.0001 (5)	0.0002 (5)	0.0012 (5)

Geometric parameters (Å, º)

O1A—C8A	1.422 (2)	C6C—H6C	0.9500
O1B—C8B	1.4492 (16)	C8C—C9C	1.4901 (18)
O1C—C8C	1.4389 (16)	C8C—H8C1	0.9900
O1D—C8D	1.4444 (17)	C8C—H8C2	0.9900
O1E—C8E	1.4490 (16)	C9C—C10C	1.3487 (18)
O1F—C8F	1.4463 (16)	C10C—C11C	1.4845 (19)
O3A—C11A	1.4136 (17)	C11C—H11E	0.9900
O3B—C11B	1.4108 (17)	C11C—H11F	0.9900
O3C—C11C	1.4249 (16)	Cl1D—C3D	1.7365 (14)
O3D—C11D	1.4214 (16)	O1D—C7D	1.3743 (17)
O3E—C11E	1.4236 (17)	O2D—C10D	1.3620 (16)
O3F—C11F	1.4121 (18)	O2D—N1D	1.4114 (14)
Cl1A—C3A	1.7320 (13)	O3D—H3OD	0.79 (2)
O1A—C7A	1.381 (2)	N1D—C1D	1.3199 (16)
O1X—C7A	1.360 (7)	C1D—C9D	1.4236 (18)
O1X—C8A	1.431 (6)	C1D—C2D	1.4654 (18)
O2A—C10A	1.3585 (15)	C2D—C3D	1.4008 (18)
O2A—N1A	1.4193 (14)	C2D—C7D	1.4123 (18)
O3A—H3OA	0.82 (2)	C3D—C4D	1.3861 (19)
N1A—C1A	1.3197 (16)	C4D—C5D	1.391 (2)
C1A—C9A	1.4218 (17)	C4D—H4D	0.9500

C1A—C2A	1.4599 (17)	C5D—C6D	1.387 (2)
C2A—C3A	1.4015 (18)	C5D—H5D	0.9500
C2A—C7A	1.4093 (18)	C6D—C7D	1.3879 (19)
C3A—C4A	1.3878 (18)	C6D—H6D	0.9500
C4A—C5A	1.388 (2)	C8D—C9D	1.4915 (18)
C4A—H4A	0.9500	C8D—H8D1	0.9900
C5A—C6A	1.384 (2)	C8D—H8D2	0.9900
C5A—H5A	0.9500	C9D—C10D	1.3521 (18)
C6A—C7A	1.3950 (19)	C10D—C11D	1.4851 (19)
C6A—H6A	0.9500	C11D—H11G	0.9900
C8A—C9A	1.4808 (18)	C11D—H11H	0.9900
C8A—H8A1	0.9900	Cl1E—C3E	1.7386 (13)
C8A—H8A2	0.9900	O1E—C7E	1.3747 (16)
C8A—H8X1	0.9900	O2E—C10E	1.3583 (15)
C8A—H8X2	0.9900	O2E—N1E	1.4140 (14)
C9A—C10A	1.3512 (17)	O3E—H3OE	0.81 (2)
C10A—C11A	1.4924 (18)	N1E—C1E	1.3182 (16)
C11A—H11A	0.9900	C1E—C9E	1.4216 (18)
C11A—H11B	0.9900	C1E—C2E	1.4638 (17)
Cl1B—C3B	1.7352 (13)	C2E—C3E	1.3996 (18)
O1B—C7B	1.3685 (16)	C2E—C7E	1.4152 (17)
O2B—C10B	1.3576 (15)	C3E—C4E	1.3882 (18)
O2B—N1B	1.4174 (14)	C4E—C5E	1.3953 (19)
O3B—H3OB	0.82 (2)	C4E—H4E	0.9500
N1B—C1B	1.3196 (16)	C5E—C6E	1.384 (2)
C1B—C9B	1.4229 (17)	C5E—H5E	0.9500
C1B—C2B	1.4611 (17)	C6E—C7E	1.4002 (17)
C2B—C3B	1.4036 (17)	C6E—H6E	0.9500
C2B—C7B	1.4076 (17)	C8E—C9E	1.4935 (17)
C3B—C4B	1.3851 (18)	C8E—H8E1	0.9900
C4B—C5B	1.389 (2)	C8E—H8E2	0.9900
C4B—H4B	0.9500	C9E—C10E	1.3554 (17)
C5B—C6B	1.388 (2)	C10E—C11E	1.4872 (19)
C5B—H5B	0.9500	C11E—H11I	0.9900
C6B—C7B	1.3966 (18)	C11E—H11J	0.9900
C6B—H6B	0.9500	Cl1F—C3F	1.7324 (13)
C8B—C9B	1.4841 (18)	O1F—C7F	1.3662 (16)
C8B—H8B1	0.9900	O2F—C10F	1.3547 (16)
C8B—H8B2	0.9900	O2F—N1F	1.4163 (14)
C9B—C10B	1.3542 (17)	O3F—H3OF	0.77 (2)
C10B—C11B	1.4948 (18)	N1F—C1F	1.3197 (16)
C11B—H11C	0.9900	C1F—C9F	1.4223 (17)
C11B—H11D	0.9900	C1F—C2F	1.4613 (18)
Cl1C—C3C	1.7368 (13)	C2F—C3F	1.4026 (18)
O1C—C7C	1.3755 (16)	C2F—C7F	1.4141 (18)
O2C—C10C	1.3584 (16)	C3F—C4F	1.3862 (19)
O2C—N1C	1.4093 (14)	C4F—C5F	1.393 (2)
O3C—H3OC	0.79 (2)	C4F—H4F	0.9500
N1C—C1C	1.3224 (16)	C5F—C6F	1.388 (2)

C1C—C9C	1.4229 (18)	C5F—H5F	0.9500
C1C—C2C	1.4605 (17)	C6F—C7F	1.3907 (18)
C2C—C3C	1.3982 (18)	C6F—H6F	0.9500
C2C—C7C	1.4140 (17)	C8F—C9F	1.4862 (18)
C3C—C4C	1.3868 (19)	C8F—H8F1	0.9900
C4C—C5C	1.393 (2)	C8F—H8F2	0.9900
C4C—H4C	0.9500	C9F—C10F	1.3545 (18)
C5C—C6C	1.387 (2)	C10F—C11F	1.4949 (19)
C5C—H5C	0.9500	C11F—H11K	0.9900
C6C—C7C	1.3929 (18)	C11F—H11L	0.9900

C7A—O1A—C8A	119.85 (19)	C9C—C10C—O2C	109.45 (11)
C7A—O1X—C8A	120.7 (7)	C9C—C10C—C11C	133.85 (13)
C10A—O2A—N1A	108.74 (9)	O2C—C10C—C11C	116.69 (11)
C11A—O3A—H3OA	109.0 (16)	O3C—C11C—C10C	109.42 (11)
C1A—N1A—O2A	104.97 (10)	O3C—C11C—H11E	109.8
N1A—C1A—C9A	111.83 (11)	C10C—C11C—H11E	109.8
N1A—C1A—C2A	128.59 (11)	O3C—C11C—H11F	109.8
C9A—C1A—C2A	119.57 (11)	C10C—C11C—H11F	109.8
C3A—C2A—C7A	116.93 (11)	H11E—C11C—H11F	108.2
C3A—C2A—C1A	127.48 (11)	C7D—O1D—C8D	118.66 (10)
C7A—C2A—C1A	115.57 (11)	C10D—O2D—N1D	109.45 (10)
C4A—C3A—C2A	122.05 (12)	C11D—O3D—H3OD	106.3 (17)
C4A—C3A—Cl1A	117.21 (10)	C1D—N1D—O2D	104.47 (10)
C2A—C3A—Cl1A	120.74 (10)	N1D—C1D—C9D	112.30 (11)
C3A—C4A—C5A	119.45 (13)	N1D—C1D—C2D	128.00 (12)
C3A—C4A—H4A	120.3	C9D—C1D—C2D	119.70 (11)
C5A—C4A—H4A	120.3	C3D—C2D—C7D	117.53 (12)
C6A—C5A—C4A	120.44 (13)	C3D—C2D—C1D	126.93 (12)
C6A—C5A—H5A	119.8	C7D—C2D—C1D	115.55 (11)
C4A—C5A—H5A	119.8	C4D—C3D—C2D	121.93 (12)
C5A—C6A—C7A	119.68 (13)	C4D—C3D—Cl1D	117.75 (11)
C5A—C6A—H6A	120.2	C2D—C3D—Cl1D	120.29 (10)
C7A—C6A—H6A	120.2	C3D—C4D—C5D	118.85 (13)
O1X—C7A—O1A	27.6 (6)	C3D—C4D—H4D	120.6
O1X—C7A—C6A	112.2 (3)	C5D—C4D—H4D	120.6
O1A—C7A—C6A	115.79 (13)	C6D—C5D—C4D	121.18 (13)
O1X—C7A—C2A	122.0 (3)	C6D—C5D—H5D	119.4
O1A—C7A—C2A	122.43 (13)	C4D—C5D—H5D	119.4
C6A—C7A—C2A	121.39 (13)	C5D—C6D—C7D	119.37 (13)
O1A—C8A—O1X	26.5 (6)	C5D—C6D—H6D	120.3
O1A—C8A—C9A	111.68 (12)	C7D—C6D—H6D	120.3
O1X—C8A—C9A	113.1 (3)	O1D—C7D—C6D	116.25 (12)
O1A—C8A—H8A1	109.3	O1D—C7D—C2D	122.44 (12)
O1X—C8A—H8A1	84.6	C6D—C7D—C2D	121.12 (13)
C9A—C8A—H8A1	109.3	O1D—C8D—C9D	110.40 (11)
O1A—C8A—H8A2	109.3	O1D—C8D—H8D1	109.6
O1X—C8A—H8A2	128.3	C9D—C8D—H8D1	109.6
C9A—C8A—H8A2	109.3	O1D—C8D—H8D2	109.6

H8A1—C8A—H8A2	107.9	C9D—C8D—H8D2	109.6
O1A—C8A—H8X1	129.9	H8D1—C8D—H8D2	108.1
O1X—C8A—H8X1	109.0	C10D—C9D—C1D	104.48 (11)
C9A—C8A—H8X1	109.0	C10D—C9D—C8D	134.54 (12)
H8A1—C8A—H8X1	27.3	C1D—C9D—C8D	120.91 (12)
H8A2—C8A—H8X1	82.9	C9D—C10D—O2D	109.29 (11)
O1A—C8A—H8X2	85.5	C9D—C10D—C11D	134.35 (13)
O1X—C8A—H8X2	109.0	O2D—C10D—C11D	116.36 (12)
C9A—C8A—H8X2	109.0	O3D—C11D—C10D	109.09 (11)
H8A1—C8A—H8X2	129.4	O3D—C11D—H11G	109.9
H8A2—C8A—H8X2	26.8	C10D—C11D—H11G	109.9
H8X1—C8A—H8X2	107.8	O3D—C11D—H11H	109.9
C10A—C9A—C1A	104.75 (11)	C10D—C11D—H11H	109.9
C10A—C9A—C8A	133.22 (12)	H11G—C11D—H11H	108.3
C1A—C9A—C8A	121.91 (11)	C7E—O1E—C8E	117.82 (10)
C9A—C10A—O2A	109.71 (11)	C10E—O2E—N1E	109.45 (9)
C9A—C10A—C11A	133.79 (12)	C11E—O3E—H3OE	102.8 (14)
O2A—C10A—C11A	116.49 (11)	C1E—N1E—O2E	104.19 (10)
O3A—C11A—C10A	108.99 (11)	N1E—C1E—C9E	112.78 (11)
O3A—C11A—H11A	109.9	N1E—C1E—C2E	127.53 (12)
C10A—C11A—H11A	109.9	C9E—C1E—C2E	119.63 (11)
O3A—C11A—H11B	109.9	C3E—C2E—C7E	117.57 (11)
C10A—C11A—H11B	109.9	C3E—C2E—C1E	127.35 (11)
H11A—C11A—H11B	108.3	C7E—C2E—C1E	115.04 (11)
C7B—O1B—C8B	118.76 (10)	C4E—C3E—C2E	122.10 (12)
C10B—O2B—N1B	108.86 (9)	C4E—C3E—Cl1E	117.69 (10)
C11B—O3B—H3OB	109.2 (16)	C2E—C3E—Cl1E	120.21 (10)
C1B—N1B—O2B	104.87 (10)	C3E—C4E—C5E	118.47 (13)
N1B—C1B—C9B	112.07 (11)	C3E—C4E—H4E	120.8
N1B—C1B—C2B	128.49 (11)	C5E—C4E—H4E	120.8
C9B—C1B—C2B	119.44 (11)	C6E—C5E—C4E	121.97 (12)
C3B—C2B—C7B	117.35 (11)	C6E—C5E—H5E	119.0
C3B—C2B—C1B	127.08 (11)	C4E—C5E—H5E	119.0
C7B—C2B—C1B	115.56 (11)	C5E—C6E—C7E	118.62 (12)
C4B—C3B—C2B	121.83 (12)	C5E—C6E—H6E	120.7
C4B—C3B—Cl1B	117.41 (10)	C7E—C6E—H6E	120.7
C2B—C3B—Cl1B	120.75 (10)	O1E—C7E—C6E	116.28 (11)
C3B—C4B—C5B	119.46 (12)	O1E—C7E—C2E	122.29 (11)
C3B—C4B—H4B	120.3	C6E—C7E—C2E	121.26 (12)
C5B—C4B—H4B	120.3	O1E—C8E—C9E	109.38 (10)
C6B—C5B—C4B	120.66 (12)	O1E—C8E—H8E1	109.8
C6B—C5B—H5B	119.7	C9E—C8E—H8E1	109.8
C4B—C5B—H5B	119.7	O1E—C8E—H8E2	109.8
C5B—C6B—C7B	119.38 (13)	C9E—C8E—H8E2	109.8
C5B—C6B—H6B	120.3	H8E1—C8E—H8E2	108.2
C7B—C6B—H6B	120.3	C10E—C9E—C1E	104.06 (11)
O1B—C7B—C6B	115.66 (11)	C10E—C9E—C8E	135.66 (12)
O1B—C7B—C2B	122.99 (11)	C1E—C9E—C8E	120.28 (11)
C6B—C7B—C2B	121.30 (12)	C9E—C10E—O2E	109.51 (11)

O1B—C8B—C9B	110.18 (10)	C9E—C10E—C11E	135.14 (12)
O1B—C8B—H8B1	109.6	O2E—C10E—C11E	115.27 (11)
C9B—C8B—H8B1	109.6	O3E—C11E—C10E	107.97 (11)
O1B—C8B—H8B2	109.6	O3E—C11E—H11I	110.1
C9B—C8B—H8B2	109.6	C10E—C11E—H11I	110.1
H8B1—C8B—H8B2	108.1	O3E—C11E—H11J	110.1
C10B—C9B—C1B	104.40 (11)	C10E—C11E—H11J	110.1
C10B—C9B—C8B	134.25 (12)	H11I—C11E—H11J	108.4
C1B—C9B—C8B	121.24 (11)	C7F—O1F—C8F	118.90 (10)
C9B—C10B—O2B	109.79 (11)	C10F—O2F—N1F	108.98 (10)
C9B—C10B—C11B	134.18 (12)	C11F—O3F—H3OF	108.3 (17)
O2B—C10B—C11B	116.00 (11)	C1F—N1F—O2F	104.82 (10)
O3B—C11B—C10B	111.18 (11)	N1F—C1F—C9F	112.03 (11)
O3B—C11B—H11C	109.4	N1F—C1F—C2F	128.30 (11)
C10B—C11B—H11C	109.4	C9F—C1F—C2F	119.63 (11)
O3B—C11B—H11D	109.4	C3F—C2F—C7F	116.97 (12)
C10B—C11B—H11D	109.4	C3F—C2F—C1F	127.36 (11)
H11C—C11B—H11D	108.0	C7F—C2F—C1F	115.63 (11)
C7C—O1C—C8C	118.28 (10)	C4F—C3F—C2F	122.22 (12)
C10C—O2C—N1C	109.41 (9)	C4F—C3F—Cl1F	117.88 (10)
C11C—O3C—H3OC	104.2 (17)	C2F—C3F—Cl1F	119.89 (10)
C1C—N1C—O2C	104.56 (10)	C3F—C4F—C5F	119.20 (13)
N1C—C1C—C9C	111.99 (11)	C3F—C4F—H4F	120.4
N1C—C1C—C2C	128.45 (12)	C5F—C4F—H4F	120.4
C9C—C1C—C2C	119.48 (11)	C6F—C5F—C4F	120.58 (13)
C3C—C2C—C7C	117.71 (11)	C6F—C5F—H5F	119.7
C3C—C2C—C1C	126.64 (11)	C4F—C5F—H5F	119.7
C7C—C2C—C1C	115.61 (11)	C5F—C6F—C7F	119.65 (13)
C4C—C3C—C2C	121.98 (12)	C5F—C6F—H6F	120.2
C4C—C3C—Cl1C	117.96 (10)	C7F—C6F—H6F	120.2
C2C—C3C—Cl1C	120.05 (10)	O1F—C7F—C6F	116.08 (12)
C3C—C4C—C5C	118.67 (13)	O1F—C7F—C2F	122.30 (12)
C3C—C4C—H4C	120.7	C6F—C7F—C2F	121.37 (12)
C5C—C4C—H4C	120.7	O1F—C8F—C9F	110.21 (10)
C6C—C5C—C4C	121.55 (13)	O1F—C8F—H8F1	109.6
C6C—C5C—H5C	119.2	C9F—C8F—H8F1	109.6
C4C—C5C—H5C	119.2	O1F—C8F—H8F2	109.6
C5C—C6C—C7C	119.01 (13)	C9F—C8F—H8F2	109.6
C5C—C6C—H6C	120.5	H8F1—C8F—H8F2	108.1
C7C—C6C—H6C	120.5	C10F—C9F—C1F	104.40 (11)
O1C—C7C—C6C	115.90 (11)	C10F—C9F—C8F	134.93 (12)
O1C—C7C—C2C	122.86 (11)	C1F—C9F—C8F	120.66 (11)
C6C—C7C—C2C	121.08 (12)	C9F—C10F—O2F	109.76 (11)
O1C—C8C—C9C	110.57 (11)	C9F—C10F—C11F	134.67 (12)
O1C—C8C—H8C1	109.5	O2F—C10F—C11F	115.56 (11)
C9C—C8C—H8C1	109.5	O3F—C11F—C10F	110.80 (12)
O1C—C8C—H8C2	109.5	O3F—C11F—H11K	109.5
C9C—C8C—H8C2	109.5	C10F—C11F—H11K	109.5
H8C1—C8C—H8C2	108.1	O3F—C11F—H11L	109.5

C10C—C9C—C1C	104.59 (11)	C10F—C11F—H11L	109.5
C10C—C9C—C8C	134.88 (12)	H11K—C11F—H11L	108.1
C1C—C9C—C8C	120.52 (11)		
C10A—O2A—N1A—C1A	−0.38 (13)	C1C—C9C—C10C—C11C	−178.04 (14)
O2A—N1A—C1A—C9A	0.71 (14)	C8C—C9C—C10C—C11C	3.4 (3)
O2A—N1A—C1A—C2A	−178.21 (12)	N1C—O2C—C10C—C9C	−0.79 (14)
N1A—C1A—C2A—C3A	4.1 (2)	N1C—O2C—C10C—C11C	178.23 (11)
C9A—C1A—C2A—C3A	−174.78 (12)	C9C—C10C—C11C—O3C	−104.66 (17)
N1A—C1A—C2A—C7A	−177.58 (13)	O2C—C10C—C11C—O3C	76.62 (15)
C9A—C1A—C2A—C7A	3.57 (17)	C10D—O2D—N1D—C1D	−0.64 (13)
C7A—C2A—C3A—C4A	−2.34 (18)	O2D—N1D—C1D—C9D	0.68 (14)
C1A—C2A—C3A—C4A	175.99 (12)	O2D—N1D—C1D—C2D	−179.61 (12)
C7A—C2A—C3A—Cl1A	177.42 (10)	N1D—C1D—C2D—C3D	8.9 (2)
C1A—C2A—C3A—Cl1A	−4.25 (18)	C9D—C1D—C2D—C3D	−171.38 (12)
C2A—C3A—C4A—C5A	0.72 (19)	N1D—C1D—C2D—C7D	−171.45 (13)
Cl1A—C3A—C4A—C5A	−179.05 (10)	C9D—C1D—C2D—C7D	8.24 (17)
C3A—C4A—C5A—C6A	0.9 (2)	C7D—C2D—C3D—C4D	−0.8 (2)
C4A—C5A—C6A—C7A	−0.7 (2)	C1D—C2D—C3D—C4D	178.85 (13)
C8A—O1X—C7A—O1A	−65.5 (12)	C7D—C2D—C3D—Cl1D	177.34 (10)
C8A—O1X—C7A—C6A	−169.0 (10)	C1D—C2D—C3D—Cl1D	−3.04 (19)
C8A—O1X—C7A—C2A	34.2 (18)	C2D—C3D—C4D—C5D	−0.2 (2)
C8A—O1A—C7A—O1X	65.3 (6)	Cl1D—C3D—C4D—C5D	−178.37 (11)
C8A—O1A—C7A—C6A	154.3 (3)	C3D—C4D—C5D—C6D	0.5 (2)
C8A—O1A—C7A—C2A	−32.8 (5)	C4D—C5D—C6D—C7D	0.2 (2)
C5A—C6A—C7A—O1X	−158.0 (9)	C8D—O1D—C7D—C6D	150.90 (13)
C5A—C6A—C7A—O1A	172.0 (2)	C8D—O1D—C7D—C2D	−34.17 (18)
C5A—C6A—C7A—C2A	−1.0 (2)	C5D—C6D—C7D—O1D	173.75 (13)
C3A—C2A—C7A—O1X	157.2 (9)	C5D—C6D—C7D—C2D	−1.3 (2)
C1A—C2A—C7A—O1X	−21.3 (9)	C3D—C2D—C7D—O1D	−173.18 (12)
C3A—C2A—C7A—O1A	−170.1 (3)	C1D—C2D—C7D—O1D	7.16 (19)
C1A—C2A—C7A—O1A	11.4 (3)	C3D—C2D—C7D—C6D	1.51 (19)
C3A—C2A—C7A—C6A	2.47 (19)	C1D—C2D—C7D—C6D	−178.15 (12)
C1A—C2A—C7A—C6A	−176.06 (12)	C7D—O1D—C8D—C9D	41.39 (16)
C7A—O1A—C8A—O1X	−63.7 (6)	N1D—C1D—C9D—C10D	−0.48 (15)
C7A—O1A—C8A—C9A	34.9 (4)	C2D—C1D—C9D—C10D	179.78 (11)
C7A—O1X—C8A—O1A	66.6 (13)	N1D—C1D—C9D—C8D	−177.76 (12)
C7A—O1X—C8A—C9A	−26.0 (17)	C2D—C1D—C9D—C8D	2.50 (18)
N1A—C1A—C9A—C10A	−0.78 (14)	O1D—C8D—C9D—C10D	157.63 (14)
C2A—C1A—C9A—C10A	178.25 (11)	O1D—C8D—C9D—C1D	−26.06 (17)
N1A—C1A—C9A—C8A	−177.31 (12)	C1D—C9D—C10D—O2D	0.05 (14)
C2A—C1A—C9A—C8A	1.72 (18)	C8D—C9D—C10D—O2D	176.78 (14)
O1A—C8A—C9A—C10A	164.6 (2)	C1D—C9D—C10D—C11D	−179.74 (14)
O1X—C8A—C9A—C10A	−166.8 (9)	C8D—C9D—C10D—C11D	−3.0 (3)
O1A—C8A—C9A—C1A	−20.0 (3)	N1D—O2D—C10D—C9D	0.36 (14)
O1X—C8A—C9A—C1A	8.6 (9)	N1D—O2D—C10D—C11D	−179.81 (11)
C1A—C9A—C10A—O2A	0.51 (14)	C9D—C10D—C11D—O3D	−108.84 (17)
C8A—C9A—C10A—O2A	176.46 (14)	O2D—C10D—C11D—O3D	71.38 (15)
C1A—C9A—C10A—C11A	−178.22 (13)	C10E—O2E—N1E—C1E	−0.65 (13)

C8A—C9A—C10A—C11A	−2.3 (3)	O2E—N1E—C1E—C9E	1.28 (14)
N1A—O2A—C10A—C9A	−0.10 (14)	O2E—N1E—C1E—C2E	178.31 (12)
N1A—O2A—C10A—C11A	178.87 (10)	N1E—C1E—C2E—C3E	15.8 (2)
C9A—C10A—C11A—O3A	1.1 (2)	C9E—C1E—C2E—C3E	−167.35 (12)
O2A—C10A—C11A—O3A	−177.53 (10)	N1E—C1E—C2E—C7E	−161.79 (13)
C10B—O2B—N1B—C1B	−0.28 (13)	C9E—C1E—C2E—C7E	15.06 (17)
O2B—N1B—C1B—C9B	0.60 (13)	C7E—C2E—C3E—C4E	1.33 (19)
O2B—N1B—C1B—C2B	179.88 (11)	C1E—C2E—C3E—C4E	−176.21 (12)
N1B—C1B—C2B—C3B	10.9 (2)	C7E—C2E—C3E—Cl1E	−178.33 (9)
C9B—C1B—C2B—C3B	−169.83 (12)	C1E—C2E—C3E—Cl1E	4.13 (18)
N1B—C1B—C2B—C7B	−170.13 (12)	C2E—C3E—C4E—C5E	−0.2 (2)
C9B—C1B—C2B—C7B	9.09 (16)	Cl1E—C3E—C4E—C5E	179.42 (10)
C7B—C2B—C3B—C4B	−0.60 (18)	C3E—C4E—C5E—C6E	−0.6 (2)
C1B—C2B—C3B—C4B	178.31 (12)	C4E—C5E—C6E—C7E	0.3 (2)
C7B—C2B—C3B—Cl1B	−179.73 (9)	C8E—O1E—C7E—C6E	151.01 (11)
C1B—C2B—C3B—Cl1B	−0.82 (18)	C8E—O1E—C7E—C2E	−33.66 (17)
C2B—C3B—C4B—C5B	−0.46 (19)	C5E—C6E—C7E—O1E	176.26 (11)
Cl1B—C3B—C4B—C5B	178.69 (10)	C5E—C6E—C7E—C2E	0.88 (19)
C3B—C4B—C5B—C6B	1.1 (2)	C3E—C2E—C7E—O1E	−176.75 (11)
C4B—C5B—C6B—C7B	−0.6 (2)	C1E—C2E—C7E—O1E	1.09 (17)
C8B—O1B—C7B—C6B	150.88 (11)	C3E—C2E—C7E—C6E	−1.65 (18)
C8B—O1B—C7B—C2B	−31.71 (17)	C1E—C2E—C7E—C6E	176.19 (11)
C5B—C6B—C7B—O1B	176.94 (11)	C7E—O1E—C8E—C9E	45.73 (15)
C5B—C6B—C7B—C2B	−0.52 (19)	N1E—C1E—C9E—C10E	−1.44 (15)
C3B—C2B—C7B—O1B	−176.18 (11)	C2E—C1E—C9E—C10E	−178.73 (11)
C1B—C2B—C7B—O1B	4.79 (17)	N1E—C1E—C9E—C8E	177.74 (12)
C3B—C2B—C7B—C6B	1.10 (18)	C2E—C1E—C9E—C8E	0.44 (18)
C1B—C2B—C7B—C6B	−177.94 (11)	O1E—C8E—C9E—C10E	149.36 (15)
C7B—O1B—C8B—C9B	40.50 (15)	O1E—C8E—C9E—C1E	−29.49 (16)
N1B—C1B—C9B—C10B	−0.71 (14)	C1E—C9E—C10E—O2E	0.95 (14)
C2B—C1B—C9B—C10B	179.95 (11)	C8E—C9E—C10E—O2E	−178.03 (14)
N1B—C1B—C9B—C8B	−177.38 (11)	C1E—C9E—C10E—C11E	−175.36 (15)
C2B—C1B—C9B—C8B	3.27 (17)	C8E—C9E—C10E—C11E	5.7 (3)
O1B—C8B—C9B—C10B	157.70 (14)	N1E—O2E—C10E—C9E	−0.24 (14)
O1B—C8B—C9B—C1B	−26.79 (16)	N1E—O2E—C10E—C11E	176.89 (11)
C1B—C9B—C10B—O2B	0.50 (14)	C9E—C10E—C11E—O3E	14.2 (2)
C8B—C9B—C10B—O2B	176.53 (13)	O2E—C10E—C11E—O3E	−161.96 (11)
C1B—C9B—C10B—C11B	−177.46 (14)	C10F—O2F—N1F—C1F	−0.97 (13)
C8B—C9B—C10B—C11B	−1.4 (3)	O2F—N1F—C1F—C9F	0.71 (14)
N1B—O2B—C10B—C9B	−0.16 (14)	O2F—N1F—C1F—C2F	178.25 (12)
N1B—O2B—C10B—C11B	178.21 (10)	N1F—C1F—C2F—C3F	10.6 (2)
C9B—C10B—C11B—O3B	−9.0 (2)	C9F—C1F—C2F—C3F	−171.99 (12)
O2B—C10B—C11B—O3B	173.12 (11)	N1F—C1F—C2F—C7F	−166.92 (12)
C10C—O2C—N1C—C1C	0.47 (13)	C9F—C1F—C2F—C7F	10.45 (17)
O2C—N1C—C1C—C9C	−0.01 (14)	C7F—C2F—C3F—C4F	0.24 (18)
O2C—N1C—C1C—C2C	−176.90 (12)	C1F—C2F—C3F—C4F	−177.29 (12)
N1C—C1C—C2C—C3C	−10.9 (2)	C7F—C2F—C3F—Cl1F	179.01 (9)
C9C—C1C—C2C—C3C	172.43 (12)	C1F—C2F—C3F—Cl1F	1.48 (18)
N1C—C1C—C2C—C7C	166.83 (13)	C2F—C3F—C4F—C5F	−0.20 (19)

C9C—C1C—C2C—C7C	−9.87 (17)	Cl1F—C3F—C4F—C5F	−179.00 (10)
C7C—C2C—C3C—C4C	0.49 (19)	C3F—C4F—C5F—C6F	−0.3 (2)
C1C—C2C—C3C—C4C	178.14 (13)	C4F—C5F—C6F—C7F	0.8 (2)
C7C—C2C—C3C—Cl1C	179.53 (10)	C8F—O1F—C7F—C6F	153.31 (12)
C1C—C2C—C3C—Cl1C	−2.81 (19)	C8F—O1F—C7F—C2F	−32.25 (18)
C2C—C3C—C4C—C5C	−0.2 (2)	C5F—C6F—C7F—O1F	173.71 (12)
Cl1C—C3C—C4C—C5C	−179.24 (10)	C5F—C6F—C7F—C2F	−0.8 (2)
C3C—C4C—C5C—C6C	−0.3 (2)	C3F—C2F—C7F—O1F	−173.89 (12)
C4C—C5C—C6C—C7C	0.3 (2)	C1F—C2F—C7F—O1F	3.93 (18)
C8C—O1C—C7C—C6C	−153.54 (12)	C3F—C2F—C7F—C6F	0.26 (18)
C8C—O1C—C7C—C2C	30.87 (18)	C1F—C2F—C7F—C6F	178.09 (12)
C5C—C6C—C7C—O1C	−175.67 (12)	C7F—O1F—C8F—C9F	42.00 (16)
C5C—C6C—C7C—C2C	0.00 (19)	N1F—C1F—C9F—C10F	−0.20 (14)
C3C—C2C—C7C—O1C	174.97 (12)	C2F—C1F—C9F—C10F	−177.98 (11)
C1C—C2C—C7C—O1C	−2.94 (18)	N1F—C1F—C9F—C8F	−179.63 (11)
C3C—C2C—C7C—C6C	−0.40 (19)	C2F—C1F—C9F—C8F	2.60 (17)
C1C—C2C—C7C—C6C	−178.31 (12)	O1F—C8F—C9F—C10F	153.38 (14)
C7C—O1C—C8C—C9C	−41.90 (16)	O1F—C8F—C9F—C1F	−27.41 (16)
N1C—C1C—C9C—C10C	−0.46 (15)	C1F—C9F—C10F—O2F	−0.43 (14)
C2C—C1C—C9C—C10C	176.75 (11)	C8F—C9F—C10F—O2F	178.87 (13)
N1C—C1C—C9C—C8C	178.39 (12)	C1F—C9F—C10F—C11F	178.69 (14)
C2C—C1C—C9C—C8C	−4.40 (18)	C8F—C9F—C10F—C11F	−2.0 (3)
O1C—C8C—C9C—C10C	−152.37 (15)	N1F—O2F—C10F—C9F	0.88 (14)
O1C—C8C—C9C—C1C	29.21 (17)	N1F—O2F—C10F—C11F	−178.42 (11)
C1C—C9C—C10C—O2C	0.74 (14)	C9F—C10F—C11F—O3F	−5.0 (2)
C8C—C9C—C10C—O2C	−177.86 (14)	O2F—C10F—C11F—O3F	174.06 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*A*—H3*OA*···O3*E*^{i}	0.82 (2)	1.99 (2)	2.8006 (14)	165 (2)
O3*B*—H3*OB*···O3*C*	0.82 (2)	1.93 (2)	2.7321 (15)	167 (2)
O3*F*—H3*OF*···O3*D*^{ii}	0.77 (2)	1.99 (2)	2.7535 (15)	170 (2)
O3*C*—H3*OC*···Cl1*A*^{iii}	0.79 (2)	2.73 (2)	3.2601 (11)	126 (2)
O3*D*—H3*OD*···Cl1*B*^{iii}	0.79 (2)	2.83 (2)	3.3070 (11)	120.7 (19)
O3*E*—H3*OE*···Cl1*F*	0.81 (2)	2.89 (2)	3.3580 (11)	118.8 (16)
O3*C*—H3*OC*···N1*A*^{iii}	0.79 (2)	2.10 (2)	2.8471 (15)	158 (2)
O3*D*—H3*OD*···N1*B*^{iii}	0.79 (2)	2.04 (2)	2.8110 (15)	165 (2)
O3*E*—H3*OE*···N1*F*	0.81 (2)	2.04 (2)	2.8132 (15)	160 (2)
C4*A*—H4*A*···O2*E*^{iv}	0.95	2.48	3.3964 (17)	162
C4*B*—H4*B*···O2*D*^{v}	0.95	2.44	3.3457 (16)	160
C4*F*—H4*F*···O2*C*^{vi}	0.95	2.61	3.4190 (17)	144
C8*A*—H8*A*1···O1*A*^{vii}	0.99	2.51	3.122 (3)	120
C8*D*—H8*D*2···O1*D*^{viii}	0.99	2.61	3.3164 (16)	128
C8*F*—H8*F*2···O1*B*^{ix}	0.99	2.60	3.2861 (16)	127
C6*C*—H6*C*···O3*A*^{i}	0.95	2.55	3.4748 (17)	164

C6*E*—H6*E*···O3*B*	0.95	2.36	3.2748 (17)	161
C11*E*—H11*I*···O1*B*^{vi}	0.99	2.53	3.2632 (16)	131

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

Selected geometric parameters (Å, °) for (II)

Molecule	O1—C8	O3—C11	O2—C10—C11—O3	C7—O1—C8—C9
A	1.422 (2)	1.4136 (17)	-177.53 (10)	34.9 (4)
B	1.4492 (16)	1.4108 (17)	173.12 (11)	40.50 (15)
C	1.4389 (16)	1.4249 (16)	76.62 (15)	-41.90 (16)
D	1.4444 (17)	1.4214 (16)	71.38 (15)	41.39 (16)
E	1.4490 (16)	1.4236 (17)	-161.96 (11)	45.73 (15)
F	1.4463 (16)	1.4121 (18)	174.06 (11)	42.00 (16)