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Crystal structure of fucoxanthin: resolving a long-standing crystallographic challenge

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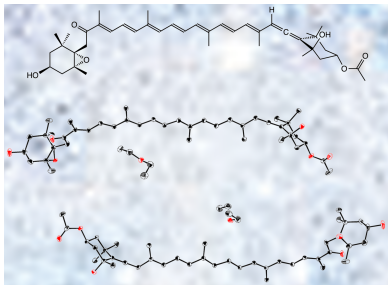
Fucoxanthin ($C_{42}H_{58}O_6$) is a highly functionalized allenic epoxy xanthophyll containing hydroxy, acetoxy, ketone and conjugated polyene units. Although its constitution and stereochemistry had been established by chemical, spectroscopic and synthetic studies, its small-molecule single-crystal X-ray structure has remained unavailable. Moss reported in 1979 [*Pure Appl. Chem.* (1979), **51**, 507–514] that an early X-ray study by G. M. Sheldrick had reached only a partial solution of the fucoxanthin structure and that refinement had stalled at $R \simeq 25\%$. The first small-molecule single-crystal X-ray structure of fucoxanthin has now been determined as the diethyl ether monosolvate, $C_{42}H_{58}O_6{\cdot}C_4H_{10}O$, at 100 K in the space group $P1$ using synchrotron radiation (λ = 0.4132 Å). The asymmetric unit contains two crystallographically independent fucoxanthin molecules and two diethyl ether molecules. The structure defines the relative stereochemistry, allene geometry, epoxide geometry, polyene bond-length alternation and solvate-assisted packing of fucoxanthin, and provides an independent small-molecule metrical reference for comparison with protein-bound fucoxanthin ligands.

1. Introduction

Fucoxanthin is an oxygenated C_{42} carotenoid of the xanthophyll family and one of the characteristic pigments of brown algae and diatoms (Mohibbullah *et al.*, 2022; Nogueira *et al.*, 2025). In the structural nomenclature of carotenoids, fucoxanthin is a highly functionalized β,β-carotenoid derivative containing hydroxy, acetoxy, epoxy, ketone and allenic units. It was first isolated from brown algae in the early 20th century (Willstätter & Page, 1914), and its unusual combination of functional groups has made it a persistent subject in carotenoid structural chemistry.

The constitution of fucoxanthin was established before the routine small-molecule crystallographic analysis of extended carotenoids became practical. Fucoxanthin and related pigments were reported in early chemical and spectroscopic studies (Bonnett *et al.*, 1966), and the detailed structure and reactions of fucoxanthin were subsequently formulated as 3′-acetoxy-5,6-epoxy-3,5′-dihydroxy-6′,7′-didehydro-5,6,7,8,5′,6′-hexahydro-β,β-caroten-8-one (Bonnett *et al.*, 1969). Later NMR studies of allenic carotenoids of the fucoxanthin series and of geometrical isomers of fucoxanthin provided a detailed solution-state foundation for the connectivity and *E*/*Z* geometry (Englert *et al.*, 1990; Hashimoto *et al.*, 2002; Haugan *et al.*, 1992). The first total synthesis of optically active fucoxanthin and halocynthiaxanthin further established a stereochemical reference for the natural product (Yamano *et al.*, 1995).

Historically, however, single-crystal X-ray structure determination of fucoxanthin has proved exceptionally challenging.



In his review of physicochemical and synthetic studies on carotenoids, Moss (1979) reported that Sheldrick had partially solved the fucoxanthin structure sufficiently to identify the two polyene chains, but that refinement was arrested at $R \simeq 25\%$, even with the use of restraints. This early attempt is a striking indication of the difficulty posed by a long, weakly absorbing, highly conjugated and conformationally flexible carotenoid containing epoxide, hydroxy, acetoxy and allenic functionalities. Motivated by this unresolved crystallographic problem, and mindful of Sheldrick's lasting legacy in crystallographic structure solution and refinement (Sheldrick, 2008; Sheldrick, 2015*b*; Usón & Herbst-Irmer, 2025), we reinvestigated fucoxanthin using modern single-crystal growth, crystal-handling and diffraction techniques.

Crystallographic precedents for other carotenoids demonstrate both the promise and the difficulty of this class of molecules. The crystal structures of unbound astaxanthin, canthaxanthin and zeaxanthin allowed detailed discussion of end-group conformation, conjugated-chain geometry and the effect of crystalline environment on carotenoid colour (Bartalucci *et al.*, 2007). More recent work on lutein crystal forms has illustrated the importance of polymorphism and solvation in carotenoid packing and stability (Guo *et al.*, 2021). These studies show that ordered lattices can be obtained for extended polyene pigments, but also that solvatomorphism, conformational flexibility and end-group disorder are central features of carotenoid crystal chemistry (Fig. S1 in the supporting information).

Fucoxanthin has also been observed in pigment–protein complexes, including the fucoxanthin chlorophyll a/c-binding protein from *Phaeodactylum tricornutum*. The crystal structure deposited as PDB entry 6a2w contains seven fucoxanthin ligands bound within the protein scaffold (Wang *et al.*, 2019). More recent cryo-EM structures of fucoxanthin chlorophyll a/c-binding assemblies have expanded the structural context of protein-bound fucoxanthin molecules (Kato *et al.*, 2024). These macromolecular models are indispensable for understanding binding-site geometry, but ligand geometries in protein structures are influenced by dictionary restraints, local density quality and limited ligand resolution. A high-resolution small-molecule structure is therefore needed as an independent metrical and stereochemical reference.

The structure reported here represents the first small-molecule single-crystal X-ray crystallographic determination of fucoxanthin as an isolated molecular compound, rather than as a restrained ligand model in a protein environment. The structure contains two crystallographically independent fucoxanthin molecules and two diethyl ether molecules in the asymmetric unit. It provides direct crystallographic parameters for the allenic cyclohexyl end group, the conjugated polyene/ketone segment and the 5,6-epoxy ionone end group, and it allows comparison of the solid-state conformations with a protein-bound A86 fucoxanthin conformer from PDB entry 6a2w.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{42}H_{58}O_6{\cdot}C_4H_{10}O$
M_r	733.00
Crystal system, space group	Triclinic, *P*1
Temperature (K)	100
a, *b*, *c* (Å)	7.9162 (9), 13.1285 (16), 21.944 (3)
α, β, γ (°)	101.178 (2), 99.094 (2), 96.991 (2)
V (Å^3)	2181.7 (4)
Z	2
Radiation type	Synchrotron, λ = 0.4132 Å
μ (mm^{-1})	0.03
Crystal size (mm)	0.01 × 0.01 × 0.01
Data collection	
Diffractometer	BL02B1 beamline of SPring-8 using a PILATUS 3X CdTe 1M detector (Dectris)
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.790, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	50529, 19428, 18495
R_{int}	0.062
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.049, 0.133, 1.04
No. of reflections	19428
No. of parameters	993
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.55, −0.32
Absolute structure	Flack *x* determined using 8327 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.2 (10)

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *SHELXTL* (Sheldrick, 2008).

2. Experimental

2.1. Crystallization

Fucoxanthin (TOPPAN Holdings Inc., >98%) was dissolved in anhydrous diethyl ether at 300 K. Slow evaporation under nitrogen at 300 K yielded aggregates of dark-orange needles. Crystals lose solvent within minutes in air; all manipulations were performed under ether vapour and crystals were mounted in Fomblin-Y and flash-cooled to 100 K.

2.2. Data collection and refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Data were collected at the BL02B1 beamline of SPring-8 using synchrotron radiation (λ = 0.4132 Å) and a PILATUS 3X CdTe 1M detector (Dectris). The frame images were converted to SFRM format using *Henkankun-R* (Shikama *et al.*, 2018). Data integration, structure solution with *SHELXT* (Sheldrick, 2015*a*) and subsequent refinement with *SHELXL* (Sheldrick, 2015*b*) were carried out using the *APEX3* (Bruker, 2016) suite. H atoms were treated using a combination of independent and constrained refinement. The H atoms attached to the terminal allene C atoms (H13 and H55) were located in difference

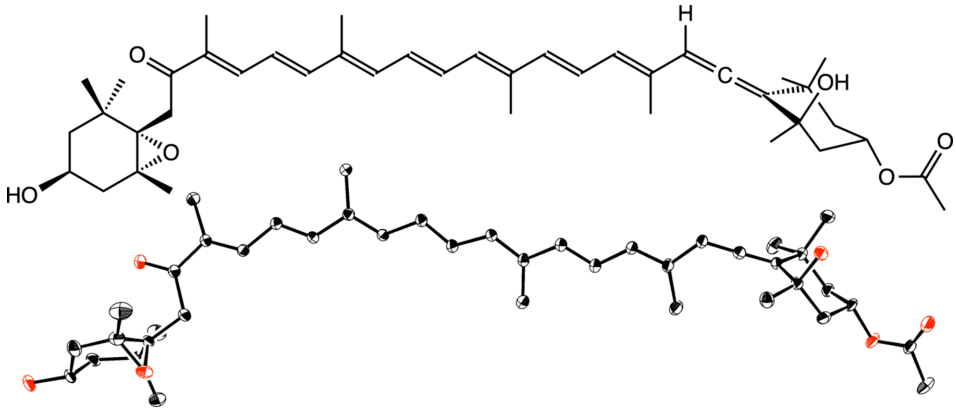


Figure 1
Chemical structure of fucoxanthin (top) and the crystal structure of fucoA (bottom) in the fucoxanthin diethyl ether monosolvate, with displacement ellipsoids drawn at the 50% probability level.

Fourier maps and refined freely. The four hydroxy H atoms H93–H96 were treated so as to allow torsional refinement of the O—H directions while retaining the standard O—H distance; the remaining H atoms were placed in calculated positions and refined using riding models. The Flack parameter refined to −0.2 (10) from 8327 Parsons quotients; because the structure contains only light atoms and was measured using high-energy radiation, the anomalous signal is not sufficient for an independent determination of the absolute structure. The absolute hand was therefore assigned by reference to the known natural product (3*S*,5*R*,6*S*,3′*S*,5′*R*,6′*R*) stereochemistry. The largest residual-density peak (0.55 e Å^{-3}) is located adjacent to the C89—C90 end of the O14-containing diethyl ether molecule and may reflect minor unresolved positional disorder of C90; no split disorder model was introduced.

3. Results and discussion

3.1. Crystal data, molecular contents and atom labelling

Fucoxanthin crystallizes as a diethyl ether monosolvate, $C_{42}H_{58}O_6{\cdot}C_4H_{10}O$, in the space group *P*1 at 100 K. The asymmetric unit contains two crystallographically independent fucoxanthin molecules and two diethyl ether molecules (Figs. 1 and 2). In the crystallographic atom labelling used here, the first fucoxanthin molecule, fucoA, comprises C1–C42 and O1–O6; the second molecule, fucoB, comprises C43–C84 and O7–O12. The solvent molecules are O13/C85–C88 and O14/C89–C92. This atom-labelling convention is used throughout the discussion. For the chemical discussion, the molecule is divided into three domains: (i) the allenic cyclohexyl end group, C1–C13/O1–O3 in fucoA and C43–C55/O7–O9 in fucoB; (ii) the conjugated polyene/ketone segment,

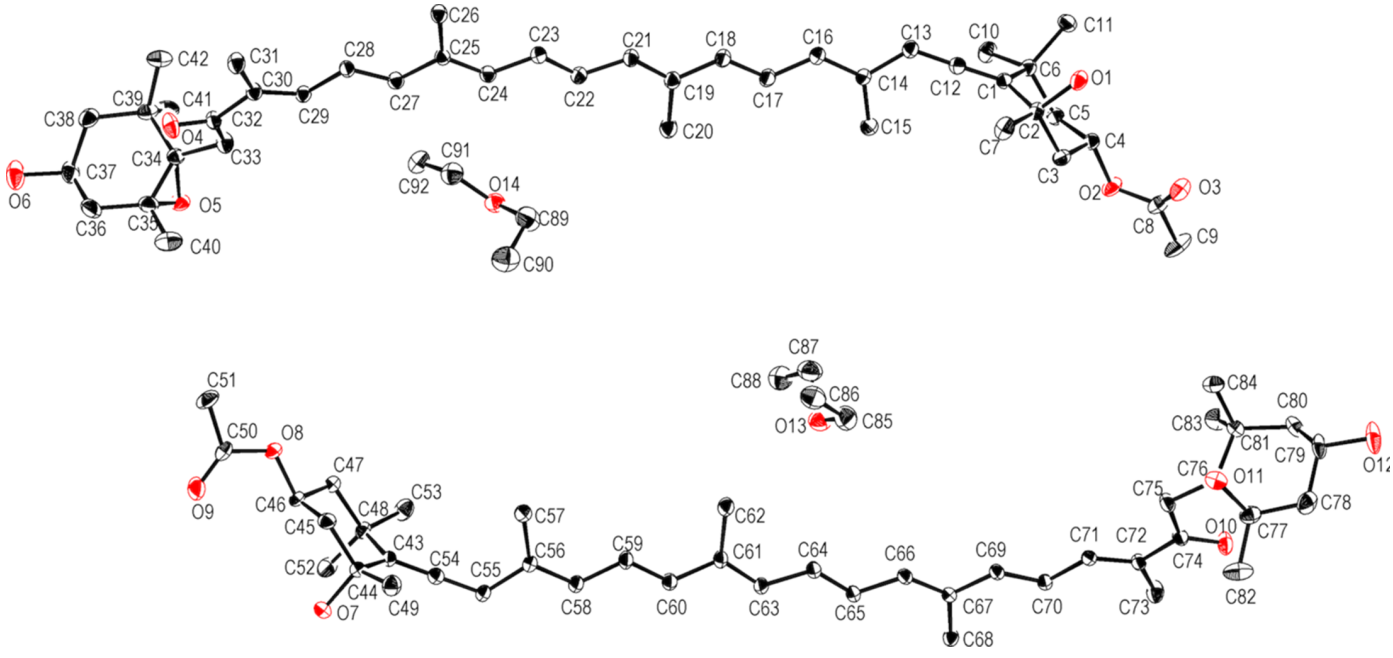


Figure 2
Packing diagram of fucoxanthin diethyl ether monosolvate with the atom labels.

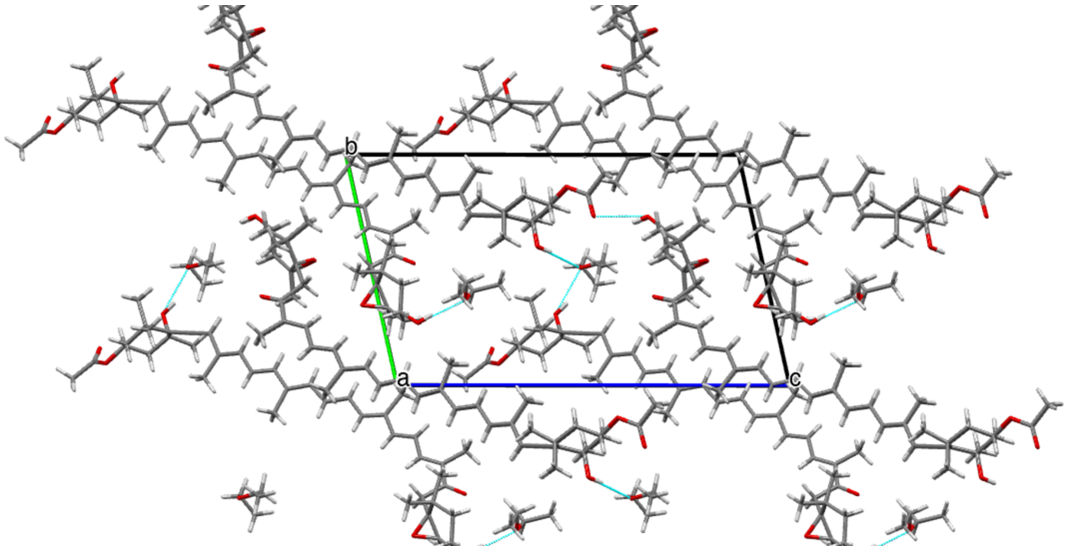


Figure 3
O—H···O hydrogen-bond contacts between fucoxanthin hydroxy groups and diethyl ether monosolvate.

C12–C33/O4 in fucoA and C54–C75/O10 in fucoB; and (iii) the 5,6-epoxy ionone end group, C32–C42/O5/O6 in fucoA and C74–C84/O11/O12 in fucoB. These structural domain names are intentionally descriptive rather than formal IUPAC substituent names; they are suitable for structural comparison of fucoxanthin and related xanthophylls.

3.2. Solvate-assisted crystal packing

Although the diethyl ether molecules are not part of the chromophore, they are not merely incidental void-filling solvent. Refinement identified four O—H···O hydrogen-bonding contacts (Table 2). In fucoA, O1—H93 and O6—H94 donate to ether atoms O14 and O13, respectively. In fucoB, O7—H95 donates to O14, whereas O12—H96 donates to acetate carbonyl atom O9 of a translation-related fucoB molecule, generating a fucoB···fucoB chain. Thus, atom O14 acts as an acceptor for two O—H···O contacts (Table 2 and Fig. 3). These contacts are best described as weak-to-moderate O—H···O hydrogen-bonding interactions (Desiraju & Steiner, 1999). The ether molecules therefore appear to assist the organization of the otherwise highly hydrophobic carotenoid framework rather than forming strong hydrogen-bonded motifs. Similar packing behaviour has been noted in related carotenoid crystal structures, where weak O—H···O and C—H···O contacts, polyene-chain stacking, end-group disorder and solvent inclusion collectively influence the packing arrangements (Bartalucci *et al.*, 2007; Guo *et al.*, 2021).

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

The C91—H91*A*···O10^{ii} contact is included for completeness; the discussion in the text focuses on the O—H···O network.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H93···O14^{i}	0.84	2.13	2.898 (2)	153
O6—H94···O13^{ii}	0.84	2.07	2.907 (3)	174
O7—H95···O14^{iii}	0.84	2.06	2.899 (2)	173
O12—H96···O9^{iv}	0.84	2.20	2.945 (3)	147
C91—H91*A*···O10^{ii}	0.99	2.60	3.589 (3)	173

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

3.3. Allenic cyclohexyl end group

The allenic cyclohexyl end group is well defined in both crystallographically independent molecules. In fucoA, the allene is C1═C12═C13, whereas the corresponding unit in fucoB is C43═C54═C55. The metrical parameters listed in Table 3 show two short C═C distances and an almost linear C═C═C angle in both molecules, as expected for an allenic unit with mutually orthogonal π-systems. The acetoxy substituent is attached through atom O2 in fucoA and through atom O8 in fucoB. Although the local acetoxy geometry is closely comparable in the two molecules, the orientation of this substituent differs between fucoA and fucoB, indicating that this end group is one of the conformationally responsive regions in the crystal. Thus, the allenic cyclohexyl end group is not simply a rigid appendage, but one of the main conformationally responsive regions in the crystal (Fig. S3 in the supporting information).

3.4. Conjugated polyene/ketone segment

The central conjugated polyene/ketone segment displays the bond-length alternation characteristic of a carotenoid π-system. The selected distances in Table 3 show that the formal C═C bonds are consistently shorter than the intervening C—C bonds in both fucoA and fucoB, while the ketone group is represented by a short C32—O4 bond in fucoA and the corresponding C74—O10 bond in fucoB. The representative torsion angles are close to 180° over most of the conjugated chain, confirming that the chromophoric framework is largely all-*E* and nearly planar in the solid state. This direct

Table 3
Selected geometrical parameters (Å, °) for the three structural domains of fucoxanthin.

Parameter/domain	fucoA	fucoB
Allenic cyclohexyl end group		
Allene C═C	C1—C12 1.308 (3); C12—C13 1.314 (3)	C43—C54 1.300 (3); C54—C55 1.317 (3)
Allene angle	C1—C12—C13 177.3 (2)	C43—C54—C55 178.4 (2)
Acetoxy C—O /O—C/C═O	C4—O2 1.460 (3); O2—C8 1.352 (3); C8—O3 1.199 (3)	C46—O8 1.468 (2); O8—C50 1.336 (3); C50—O9 1.208 (3)
Conjugated polyene/ketone segment		
Mean formal C═C in polyene chain	1.359; range 1.354–1.368	1.358; range 1.355–1.366
Mean intervening C—C in polyene chain	1.449; range 1.425–1.484	1.449; range 1.430–1.477
Ketone C═O	C32—O4 1.222 (3)	C74—O10 1.219 (3)
Representative polyene torsion angles	C12—C13—C14—C16 177.9 (2); C13—C14—C16—C17 −179.3 (2); C16—C17—C18—C19 −177.0 (2); C21—C22—C23—C24 177.6 (2)	C54—C55—C56—C58 −171.5 (2); C55—C56—C58—C59 176.8 (2); C58—C59—C60—C61 177.5 (2); C63—C64—C65—C66 −175.7 (2)
5,6-Epoxy ionone end group		
Epoxide C—O	C34—O5 1.461 (3); C35—O5 1.457 (3)	C76—O11 1.463 (3); C77—O11 1.453 (3)
Epoxide angle	C34—O5—C35 60.90 (14)	C76—O11—C77 60.85 (14)
Hydroxy C—O	C37—O6 1.430 (3)	C79—O12 1.428 (3)
Terminal-ring junction torsion angles	C30—C32—C33—C34 −163.4 (2); C32—C33—C34—C35 −77.8 (3); C33—C34—C35—C36 153.8 (2)	C72—C74—C75—C76 −179.1 (2); C74—C75—C76—C77 −71.3 (3); C75—C76—C77—C78 153.2 (2)

Note: formal C═C and intervening C—C averages were calculated from the crystallographically defined conjugated polyene segment, excluding the allene and the terminal saturated ring bonds.

crystallographic observation is consistent with the solution-state formulation derived from NMR studies of fucoxanthin and its geometrical isomers (Englert *et al.*, 1990; Hashimoto *et al.*, 2002; Haugan *et al.*, 1992). The small deviations from coplanarity are concentrated near the terminal-ring junctions rather than in the central polyene itself. Accordingly, the principal conformational variability in the crystal is associated with the terminal domains rather than with the central conjugated chain.

3.5. 5,6-Epoxy ionone end group

The 5,6-epoxy ionone end group is also well resolved in both independent molecules. In fucoA, the epoxide is C34—O5—C35, whereas the corresponding epoxide in fucoB is C76—O11—C77. The C—O distances and three-membered-ring angles listed in Table 3 are closely similar for the two molecules, indicating that the intrinsic epoxide geometry is conserved. In contrast, the torsion angles that connect this end group to the polyene/ketone segment differ between fucoA and fucoB. The local stereochemical arrangement of the epoxide-bearing ring is therefore retained, but its orientation relative to the chromophoric chain is variable. This behaviour is consistent with the role of ionone-type terminal rings as conformationally flexible end groups in xanthophyll and carotenoid crystal structures (Bartalucci *et al.*, 2007; Guo *et al.*, 2021).

3.6. Stereochemical implications and absolute structure

The present structure defines the relative stereochemistry of fucoxanthin directly in the solid state. In the atom labels used here, the stereochemically significant tetrahedral centres are C2, C4, C34, C35 and C37 in fucoA, and C44, C46, C76, C77 and C79 in fucoB, together with the allenic stereogenic axis C1═C12═C13 in fucoA and C43═C54═C55 in fucoB. The two crystallographically independent molecules have the same connectivity and relative stereochemical arrangement. The relative configuration is illustrated in Fig. S1 in the supporting information; the *R**/*S** notation there denotes relative configuration only.

Because the structure contains only light atoms and was measured at short wavelength, the refined Flack parameter [−0.2 (10)] is not decisive for absolute structure determination. The absolute hand of the model was therefore assigned by reference to the established natural product and synthetic stereochemical formulation rather than from anomalous scattering determination alone. The refined Flack parameter is statistically consistent with zero and hence with the assigned hand, although its large standard uncertainty precludes an independent absolute structure determination (Thompson & Watkin, 2011). The crystallographic model provides a direct coordinate-based validation of the relative stereochemical arrangement inferred from degradative chemistry, solution-state NMR and total synthesis (Bonnett *et al.*, 1969; Englert *et al.*, 1990; Haugan *et al.*, 1992; Yamano *et al.*, 1995).

3.7. Comparison with protein-bound A86 fucoxanthin in PDB entry 6a2w

The protein-bound fucoxanthin-A86 ligand in PDB entry 6a2w provides a useful comparison with a biologically bound fucoxanthin conformer, but its ligand geometry should not be used as a small-molecule metrical standard. The deposited structure was determined at 1.80 Å resolution and contains seven fucoxanthin molecules in the protein scaffold (Wang *et al.*, 2019). Such ligand models reflect the combined effects of local electron density, refinement restraints and protein binding interactions. Consequently, the appropriate comparison is conformational rather than metrical.

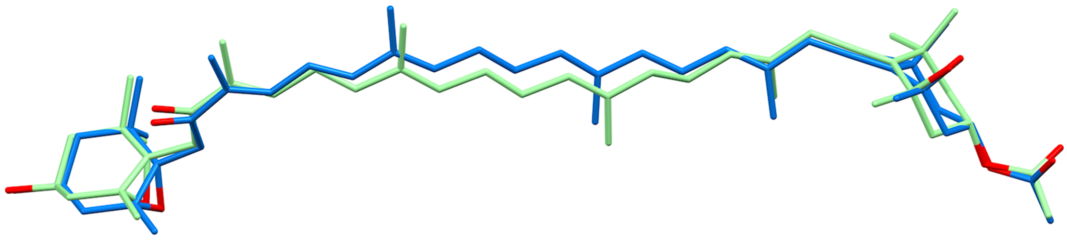


Figure 4
Overlay of protein-bound fucoxanthin-A86 residue 302 from PDB entry 6a2w with fucoA from the present small-molecule structure. A86 is shown in green, fucoA in blue and O atoms in red.

A graph-based atom correspondence followed by Kabsch superposition of fucoxanthin-A86 residue 302 against fucoA gives a heavy-atom root-mean-square deviation of 0.619 Å (Schrödinger, 2026). The corresponding comparison with fucoB is provided in Fig. S2. The comparison is intended to show conformational similarity and terminal-domain flexibility rather than to compare individual bond lengths or angles (Fig. 4). The representative A86/fucoA overlay shows that the largest deviations are localized around the terminal-ring junctions and the acetoxy/allene-containing end-group region, whereas the conjugated polyene framework is largely conserved. This comparison supports a central conclusion of the small-molecule structure: the polyene chain provides a relatively conserved structural spine, while the terminal domains accommodate substantial conformational adjustment.

4. Conclusion

The single-crystal structure of fucoxanthin diethyl ether monosolvate represents the first small-molecule single-crystal X-ray structure of this allenic epoxy xanthophyll. The structure confirms the constitution and relative stereochemical arrangement previously inferred from degradative chemistry, solution-state NMR and total synthesis, while providing direct metrical parameters for the allene, epoxide, acetoxy substituent, conjugated ketone and polyene chain. The presence of two crystallographically independent molecules shows that the polyene core is conformationally conserved, whereas both terminal end groups retain appreciable flexibility in the solid state. The diethyl ether molecules participate in the packing through O—H···O hydrogen-bonding contacts. Comparison with protein-bound A86 fucoxanthin in PDB entry 6a2w further indicates that the small-molecule structure supplies a more reliable metrical reference, while the protein-bound conformer shows the same principal pattern of conformational variation, namely, conservation of the polyene spine and flexibility of the terminal domains. The structure therefore resolves a long-standing crystallographic problem in carotenoid chemistry and supplies a benchmark for future structural discussion of fucoxanthin and related allenic epoxy xanthophylls.

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Crystal structure of fucoxanthin: resolving a long-standing crystallographic challenge

Yui Wakasa and Mao Minoura

Computing details

(1*S*,3*R*)-3-hydroxy-4-[(3*Z*,5*E*,7*Z*,9*E*,11*Z*,13*E*,15*Z*)-18-{(1*S*,4*S*,6*R*)-4-Hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]heptan-1-yl}-3,7,12,16-tetramethyl-17-oxooctadeca-1,3,5,7,9,11,13,15-octaen-1-ylidene]-3,5,5-trimethylcyclohexyl acetate

Crystal data

$C_{42}H_{58}O_6 \cdot C_4H_{10}O$
M_r = 733.00
Triclinic, $P\overline{1}$
a = 7.9162 (9) Å
b = 13.1285 (16) Å
c = 21.944 (3) Å
α = 101.178 (2)°
β = 99.094 (2)°
γ = 96.991 (2)°
V = 2181.7 (4) Å^3
Z = 2
$F(000)$ = 800
D_x = 1.116 Mg m^{-3}
Synchrotron radiation, λ = 0.4132 Å
Cell parameters from 9990 reflections
θ = 2.2–15.5°
μ = 0.03 mm^{-1}
T = 100 K
Needle, brown
0.01 × 0.01 × 0.01 mm

Data collection

Dectris PILATUS-CdTe diffractometer
Radiation source: BL02B1 SPring-8
Phi scan
Absorption correction: multi-scan SADABS
T_{min} = 0.790, T_{max} = 1.000
50529 measured reflections
19428 independent reflections
18495 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 15.6°, θ_{min} = 0.9°
h = −10→10
k = −17→17
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.133
S = 1.04
19428 reflections
993 parameters
3 restraints
Primary atom site location: SHELXT2014 (Sheldrick, 2015*a*)
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0742P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack x determined using 8327 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.2 (10)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.5585 (3)	1.23088 (16)	0.45057 (10)	0.0182 (4)
C2	1.7456 (3)	1.21336 (18)	0.44653 (10)	0.0200 (4)
C3	1.7481 (3)	1.13703 (18)	0.38445 (11)	0.0219 (4)
H3	1.8696	1.1326	0.3799	0.026*
H3A	1.6913	1.0661	0.3855	0.026*
C4	1.6551 (3)	1.17234 (17)	0.32800 (10)	0.0207 (4)
H4	1.7148	1.2424	0.3251	0.025*
C5	1.4679 (3)	1.17774 (18)	0.33307 (10)	0.0209 (4)
H5	1.4095	1.1067	0.3332	0.025*
H5A	1.4097	1.1991	0.2953	0.025*
C6	1.4451 (3)	1.25515 (17)	0.39282 (10)	0.0196 (4)
O1	1.8468 (2)	1.30932 (14)	0.44256 (8)	0.0249 (3)
H93	1.8539	1.3546	0.4761	0.037*
C7	1.8307 (3)	1.1733 (2)	0.50279 (12)	0.0302 (5)
H7	1.9492	1.1633	0.4983	0.045*
H7A	1.7639	1.1062	0.5042	0.045*
H7B	1.8338	1.2248	0.5420	0.045*
O2	1.6485 (2)	1.09495 (14)	0.26972 (8)	0.0271 (4)
C8	1.7863 (3)	1.1029 (2)	0.24056 (11)	0.0266 (5)
O3	1.9200 (2)	1.16115 (16)	0.26277 (9)	0.0320 (4)
C9	1.7477 (4)	1.0294 (3)	0.17667 (13)	0.0418 (7)
H9	1.7304	1.0699	0.1437	0.063*
H9A	1.6425	0.9793	0.1733	0.063*
H9B	1.8452	0.9912	0.1714	0.063*
C10	1.2528 (3)	1.2385 (2)	0.39726 (12)	0.0268 (5)
H10	1.2333	1.2893	0.4336	0.040*
H10A	1.2187	1.1669	0.4026	0.040*
H10B	1.1832	1.2487	0.3584	0.040*
C11	1.4979 (3)	1.36963 (18)	0.38788 (11)	0.0258 (5)
H11	1.4201	1.3850	0.3526	0.039*
H11A	1.6172	1.3795	0.3806	0.039*
H11B	1.4899	1.4173	0.4273	0.039*
C12	1.4957 (3)	1.22680 (18)	0.50185 (11)	0.0202 (4)
C13	1.4261 (3)	1.22426 (18)	0.55217 (10)	0.0212 (4)
H13	1.447 (4)	1.289 (2)	0.5860 (14)	0.020 (7)*
C14	1.3216 (3)	1.13164 (17)	0.56321 (10)	0.0196 (4)
C15	1.2842 (4)	1.03334 (19)	0.51191 (11)	0.0271 (5)
H15	1.2532	0.9725	0.5299	0.041*
H15A	1.3873	1.0248	0.4931	0.041*

H15B	1.1878	1.0387	0.4793	0.041*
C16	1.2628 (3)	1.13982 (18)	0.61845 (11)	0.0221 (4)
H16	1.2917	1.2061	0.6473	0.027*
C17	1.1602 (3)	1.05690 (19)	0.63756 (11)	0.0223 (4)
H17	1.1177	0.9928	0.6075	0.027*
C18	1.1215 (3)	1.06588 (19)	0.69616 (11)	0.0221 (4)
H18	1.1600	1.1315	0.7251	0.026*
C19	1.0262 (3)	0.98328 (18)	0.71808 (11)	0.0207 (4)
C20	0.9605 (3)	0.8799 (2)	0.67198 (11)	0.0276 (5)
H20	1.0590	0.8469	0.6605	0.041*
H20A	0.8899	0.8919	0.6339	0.041*
H20B	0.8900	0.8335	0.6915	0.041*
C21	1.0042 (3)	1.00117 (18)	0.77948 (11)	0.0208 (4)
H21	1.0522	1.0685	0.8053	0.025*
C22	0.9153 (3)	0.92747 (18)	0.80839 (11)	0.0210 (4)
H22	0.8589	0.8621	0.7820	0.025*
C23	0.9053 (3)	0.94382 (17)	0.87074 (11)	0.0208 (4)
H23	0.9638	1.0072	0.8988	0.025*
C24	0.8077 (3)	0.86657 (17)	0.89430 (10)	0.0198 (4)
H24	0.7594	0.8030	0.8644	0.024*
C25	0.7737 (3)	0.87114 (17)	0.95389 (10)	0.0182 (4)
C26	0.8452 (3)	0.96218 (18)	1.00820 (11)	0.0220 (4)
H26	0.9279	1.0118	0.9953	0.033*
H26A	0.9042	0.9368	1.0437	0.033*
H26B	0.7505	0.9975	1.0212	0.033*
C27	0.6572 (3)	0.78459 (18)	0.96338 (10)	0.0201 (4)
H27	0.6127	0.7290	0.9276	0.024*
C28	0.6045 (3)	0.77434 (17)	1.01809 (10)	0.0189 (4)
H28	0.6501	0.8261	1.0557	0.023*
C29	0.4795 (3)	0.68547 (17)	1.01964 (10)	0.0187 (4)
H29	0.4221	0.6423	0.9801	0.022*
C30	0.4366 (3)	0.65796 (18)	1.07225 (10)	0.0199 (4)
C31	0.5183 (3)	0.7140 (2)	1.13879 (11)	0.0268 (5)
H31	0.6270	0.7583	1.1385	0.040*
H31A	0.5420	0.6623	1.1645	0.040*
H31B	0.4391	0.7581	1.1568	0.040*
C32	0.3064 (3)	0.56332 (18)	1.06606 (10)	0.0213 (4)
O4	0.2878 (3)	0.52745 (16)	1.11240 (8)	0.0318 (4)
C33	0.1924 (3)	0.51115 (19)	1.00187 (11)	0.0247 (5)
H33	0.1521	0.5661	0.9806	0.030*
H33A	0.2616	0.4709	0.9749	0.030*
C34	0.0372 (3)	0.43800 (17)	1.00906 (10)	0.0202 (4)
C35	0.0622 (3)	0.33319 (18)	1.02081 (11)	0.0260 (5)
C36	−0.0598 (4)	0.2781 (2)	1.05515 (13)	0.0341 (6)
H36	−0.0039	0.2893	1.1001	0.041*
H36A	−0.0782	0.2016	1.0369	0.041*
C37	−0.2348 (4)	0.3150 (2)	1.05194 (13)	0.0328 (6)
H37	−0.2977	0.2931	1.0071	0.039*

C38	−0.2102 (3)	0.4337 (2)	1.07081 (12)	0.0295 (5)
H38	−0.1411	0.4565	1.1142	0.035*
H38A	−0.3250	0.4559	1.0717	0.035*
C39	−0.1198 (3)	0.48965 (19)	1.02660 (11)	0.0249 (5)
O5	−0.0152 (2)	0.34417 (13)	0.95809 (8)	0.0252 (3)
C40	0.2337 (4)	0.2937 (2)	1.02337 (15)	0.0398 (6)
H40	0.2138	0.2176	1.0067	0.060*
H40A	0.2957	0.3097	1.0673	0.060*
H40B	0.3031	0.3284	0.9978	0.060*
O6	−0.3359 (3)	0.26639 (19)	1.09012 (10)	0.0476 (6)
H94	−0.3082	0.3002	1.1278	0.071*
C41	−0.2457 (4)	0.4861 (2)	0.96486 (13)	0.0333 (5)
H41	−0.3434	0.5214	0.9746	0.050*
H41A	−0.2888	0.4127	0.9433	0.050*
H41B	−0.1852	0.5218	0.9374	0.050*
C42	−0.0669 (4)	0.6058 (2)	1.06153 (14)	0.0342 (6)
H42	−0.1696	0.6344	1.0725	0.051*
H42A	−0.0151	0.6461	1.0341	0.051*
H42B	0.0175	0.6107	1.1002	0.051*
C43	−0.2634 (3)	−0.26779 (16)	0.37838 (10)	0.0179 (4)
C44	−0.1751 (3)	−0.29419 (17)	0.43954 (10)	0.0193 (4)
C45	−0.2182 (3)	−0.22215 (18)	0.49746 (10)	0.0221 (4)
H45	−0.1757	−0.2471	0.5360	0.026*
H45A	−0.1570	−0.1499	0.5021	0.026*
C46	−0.4103 (3)	−0.21999 (17)	0.49171 (10)	0.0211 (4)
H46	−0.4741	−0.2910	0.4908	0.025*
C47	−0.4802 (3)	−0.18092 (17)	0.43374 (10)	0.0204 (4)
H47	−0.4213	−0.1084	0.4375	0.025*
H47A	−0.6054	−0.1786	0.4319	0.025*
C48	−0.4543 (3)	−0.25090 (18)	0.37190 (10)	0.0196 (4)
O7	−0.2448 (2)	−0.40104 (13)	0.43707 (8)	0.0229 (3)
H95	−0.1872	−0.4227	0.4662	0.034*
C49	0.0220 (3)	−0.2814 (2)	0.44528 (12)	0.0276 (5)
H49	0.0738	−0.2987	0.4849	0.041*
H49A	0.0673	−0.2086	0.4452	0.041*
H49B	0.0512	−0.3288	0.4095	0.041*
O8	−0.4350 (3)	−0.14237 (13)	0.54620 (8)	0.0269 (4)
C50	−0.4833 (3)	−0.1763 (2)	0.59536 (11)	0.0246 (5)
O9	−0.5130 (3)	−0.26788 (16)	0.59743 (10)	0.0416 (5)
C51	−0.4899 (4)	−0.0855 (2)	0.64797 (12)	0.0334 (6)
H51	−0.5981	−0.0978	0.6637	0.050*
H51A	−0.4847	−0.0206	0.6321	0.050*
H51B	−0.3912	−0.0790	0.6824	0.050*
C52	−0.5753 (3)	−0.3579 (2)	0.35751 (12)	0.0285 (5)
H52	−0.5615	−0.4002	0.3171	0.043*
H52A	−0.6958	−0.3459	0.3550	0.043*
H52B	−0.5451	−0.3952	0.3913	0.043*
C53	−0.5025 (3)	−0.1948 (2)	0.31778 (11)	0.0291 (5)

H53	−0.4210	−0.1295	0.3244	0.044*
H53A	−0.6203	−0.1785	0.3170	0.044*
H53B	−0.4970	−0.2407	0.2774	0.044*
C54	−0.1809 (3)	−0.26529 (17)	0.33184 (11)	0.0209 (4)
C55	−0.1014 (3)	−0.26264 (18)	0.28366 (11)	0.0212 (4)
H55	−0.102 (4)	−0.321 (2)	0.2511 (14)	0.020 (7)*
C56	−0.0046 (3)	−0.16774 (18)	0.27189 (10)	0.0199 (4)
C57	0.0248 (4)	−0.06939 (19)	0.32257 (11)	0.0276 (5)
H57	0.0696	−0.0094	0.3060	0.041*
H57A	0.1089	−0.0766	0.3588	0.041*
H57B	−0.0849	−0.0578	0.3360	0.041*
C58	0.0511 (3)	−0.17448 (18)	0.21614 (10)	0.0210 (4)
H58	0.0292	−0.2419	0.1885	0.025*
C59	0.1404 (3)	−0.08952 (18)	0.19445 (10)	0.0208 (4)
H59	0.1721	−0.0222	0.2221	0.025*
C60	0.1803 (3)	−0.10284 (18)	0.13591 (10)	0.0199 (4)
H60	0.1514	−0.1715	0.1097	0.024*
C61	0.2635 (3)	−0.02072 (17)	0.10992 (10)	0.0188 (4)
C62	0.3035 (3)	0.08923 (19)	0.14935 (11)	0.0251 (5)
H62	0.3649	0.1354	0.1271	0.038*
H62A	0.3765	0.0899	0.1899	0.038*
H62B	0.1953	0.1143	0.1568	0.038*
C63	0.2952 (3)	−0.04614 (17)	0.04986 (10)	0.0188 (4)
H63	0.2568	−0.1166	0.0271	0.023*
C64	0.3813 (3)	0.02440 (17)	0.01830 (10)	0.0192 (4)
H64	0.4310	0.0927	0.0424	0.023*
C65	0.3976 (3)	0.00147 (17)	−0.04339 (10)	0.0194 (4)
H65	0.3428	−0.0642	−0.0698	0.023*
C66	0.4971 (3)	0.07606 (16)	−0.06868 (10)	0.0193 (4)
H66	0.5494	0.1397	−0.0396	0.023*
C67	0.5273 (3)	0.06840 (16)	−0.12869 (10)	0.0176 (4)
C68	0.4505 (3)	−0.02354 (17)	−0.18214 (10)	0.0211 (4)
H68	0.5429	−0.0607	−0.1957	0.032*
H68A	0.3906	0.0015	−0.2177	0.032*
H68B	0.3678	−0.0715	−0.1680	0.032*
C69	0.6445 (3)	0.15355 (17)	−0.13978 (10)	0.0187 (4)
H69	0.6980	0.2070	−0.1038	0.022*
C70	0.6864 (3)	0.16551 (17)	−0.19577 (10)	0.0185 (4)
H70	0.6323	0.1159	−0.2335	0.022*
C71	0.8121 (3)	0.25271 (16)	−0.19877 (10)	0.0180 (4)
H71	0.8692	0.2973	−0.1596	0.022*
C72	0.8572 (3)	0.27751 (16)	−0.25175 (10)	0.0177 (4)
C73	0.7748 (3)	0.2182 (2)	−0.31777 (11)	0.0270 (5)
H73	0.8586	0.1794	−0.3367	0.041*
H73A	0.7390	0.2680	−0.3434	0.041*
H73B	0.6732	0.1688	−0.3161	0.041*
C74	0.9945 (3)	0.36687 (18)	−0.24746 (10)	0.0207 (4)
O10	1.0417 (3)	0.38475 (15)	−0.29512 (8)	0.0304 (4)

C75	1.0780 (3)	0.43707 (18)	−0.18270 (11)	0.0241 (4)
H75	0.9875	0.4679	−0.1623	0.029*
H75A	1.1330	0.3940	−0.1553	0.029*
C76	1.2134 (3)	0.52473 (17)	−0.18927 (10)	0.0186 (4)
C77	1.3773 (3)	0.4965 (2)	−0.20645 (12)	0.0266 (5)
C78	1.4793 (3)	0.5643 (2)	−0.24083 (14)	0.0336 (6)
H78	1.6044	0.5647	−0.2264	0.040*
H78A	1.4507	0.5324	−0.2867	0.040*
C79	1.4446 (3)	0.6759 (2)	−0.23067 (11)	0.0285 (5)
H79	1.4862	0.7094	−0.1849	0.034*
C80	1.2504 (3)	0.67632 (19)	−0.24571 (11)	0.0253 (5)
H80	1.2048	0.6366	−0.2896	0.030*
H80A	1.2294	0.7497	−0.2433	0.030*
C81	1.1505 (3)	0.62773 (17)	−0.20071 (11)	0.0206 (4)
O11	1.3718 (2)	0.54447 (13)	−0.14144 (8)	0.0254 (3)
C82	1.4153 (4)	0.3847 (2)	−0.21588 (17)	0.0436 (7)
H82	1.5395	0.3857	−0.2019	0.065*
H82A	1.3816	0.3504	−0.2608	0.065*
H82B	1.3494	0.3459	−0.1911	0.065*
O12	1.5389 (3)	0.73428 (19)	−0.26641 (10)	0.0461 (6)
H96	1.5033	0.7090	−0.3052	0.069*
C83	0.9575 (3)	0.6109 (2)	−0.22997 (14)	0.0325 (5)
H83	0.9252	0.6774	−0.2382	0.049*
H83A	0.8890	0.5863	−0.2007	0.049*
H83B	0.9350	0.5582	−0.2698	0.049*
C84	1.1739 (3)	0.70476 (19)	−0.13638 (12)	0.0271 (5)
H84	1.1305	0.7695	−0.1425	0.041*
H84A	1.2971	0.7213	−0.1170	0.041*
H84B	1.1091	0.6725	−0.1086	0.041*
O13	0.7602 (3)	0.36760 (16)	0.22348 (9)	0.0364 (4)
C85	0.9387 (4)	0.4087 (3)	0.24665 (15)	0.0413 (6)
H85	0.9680	0.4721	0.2299	0.050*
H85A	1.0088	0.3559	0.2300	0.050*
C86	0.9893 (4)	0.4375 (3)	0.31788 (15)	0.0407 (6)
H86	0.9245	0.4920	0.3348	0.061*
H86A	1.1138	0.4640	0.3300	0.061*
H86B	0.9625	0.3751	0.3350	0.061*
C87	0.6478 (4)	0.4440 (2)	0.23459 (15)	0.0391 (6)
H87	0.6731	0.5006	0.2118	0.047*
H87A	0.6661	0.4759	0.2803	0.047*
C88	0.4639 (4)	0.3903 (3)	0.21151 (14)	0.0391 (6)
H88	0.4461	0.3602	0.1660	0.059*
H88A	0.3852	0.4415	0.2194	0.059*
H88B	0.4401	0.3341	0.2340	0.059*
O14	−0.0645 (2)	0.50808 (14)	0.53382 (8)	0.0268 (3)
C89	0.1206 (4)	0.5188 (3)	0.53735 (18)	0.0426 (7)
H89	0.1739	0.5895	0.5628	0.051*
H89A	0.1453	0.5145	0.4942	0.051*

C90	0.2036 (4)	0.4389 (3)	0.56528 (18)	0.0471 (7)
H90	0.1976	0.4503	0.6103	0.071*
H90A	0.3252	0.4451	0.5604	0.071*
H90B	0.1431	0.3685	0.5436	0.071*
C91	−0.1120 (4)	0.5357 (2)	0.59371 (13)	0.0336 (5)
H91	−0.0683	0.6108	0.6128	0.040*
H91A	−0.0611	0.4931	0.6223	0.040*
C92	−0.3059 (4)	0.5155 (3)	0.58480 (15)	0.0382 (6)
H92	−0.3551	0.5590	0.5571	0.057*
H92A	−0.3412	0.5331	0.6259	0.057*
H92B	−0.3482	0.4411	0.5655	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0205 (9)	0.0169 (9)	0.0166 (9)	0.0015 (7)	0.0037 (7)	0.0027 (7)
C2	0.0190 (9)	0.0227 (10)	0.0180 (9)	0.0010 (8)	0.0055 (7)	0.0036 (8)
C3	0.0219 (10)	0.0212 (10)	0.0225 (10)	0.0049 (8)	0.0057 (8)	0.0021 (8)
C4	0.0249 (10)	0.0184 (10)	0.0168 (9)	0.0004 (8)	0.0057 (8)	−0.0004 (7)
C5	0.0231 (10)	0.0207 (10)	0.0175 (9)	0.0018 (8)	0.0030 (8)	0.0021 (8)
C6	0.0214 (10)	0.0212 (10)	0.0171 (9)	0.0043 (8)	0.0048 (8)	0.0047 (8)
O1	0.0227 (8)	0.0271 (8)	0.0210 (8)	−0.0034 (6)	0.0068 (6)	−0.0022 (6)
C7	0.0262 (11)	0.0437 (15)	0.0239 (11)	0.0118 (10)	0.0041 (9)	0.0113 (10)
O2	0.0282 (8)	0.0291 (9)	0.0192 (8)	0.0011 (7)	0.0066 (6)	−0.0062 (6)
C8	0.0282 (11)	0.0318 (12)	0.0193 (10)	0.0100 (9)	0.0054 (9)	0.0002 (9)
O3	0.0286 (9)	0.0394 (10)	0.0263 (9)	0.0044 (8)	0.0082 (7)	0.0010 (7)
C9	0.0346 (14)	0.0570 (19)	0.0260 (13)	0.0107 (13)	0.0082 (10)	−0.0136 (12)
C10	0.0215 (10)	0.0348 (13)	0.0253 (11)	0.0068 (9)	0.0048 (8)	0.0077 (9)
C11	0.0354 (12)	0.0198 (10)	0.0236 (10)	0.0050 (9)	0.0064 (9)	0.0066 (8)
C12	0.0211 (10)	0.0204 (10)	0.0188 (9)	0.0037 (8)	0.0026 (8)	0.0044 (7)
C13	0.0233 (10)	0.0223 (10)	0.0183 (10)	0.0030 (8)	0.0060 (8)	0.0040 (8)
C14	0.0228 (10)	0.0200 (10)	0.0172 (9)	0.0043 (8)	0.0061 (8)	0.0042 (8)
C15	0.0394 (13)	0.0221 (11)	0.0204 (10)	0.0039 (9)	0.0104 (9)	0.0028 (8)
C16	0.0263 (11)	0.0224 (11)	0.0188 (10)	0.0037 (8)	0.0080 (8)	0.0043 (8)
C17	0.0230 (10)	0.0248 (11)	0.0209 (10)	0.0048 (8)	0.0075 (8)	0.0060 (8)
C18	0.0231 (10)	0.0242 (11)	0.0209 (10)	0.0047 (8)	0.0077 (8)	0.0063 (8)
C19	0.0187 (9)	0.0224 (10)	0.0221 (10)	0.0037 (8)	0.0054 (8)	0.0062 (8)
C20	0.0323 (12)	0.0271 (12)	0.0218 (11)	−0.0018 (9)	0.0079 (9)	0.0030 (9)
C21	0.0197 (9)	0.0221 (10)	0.0214 (10)	0.0021 (8)	0.0061 (8)	0.0057 (8)
C22	0.0202 (10)	0.0221 (10)	0.0222 (10)	0.0044 (8)	0.0064 (8)	0.0058 (8)
C23	0.0207 (10)	0.0198 (10)	0.0222 (10)	0.0017 (8)	0.0056 (8)	0.0050 (8)
C24	0.0185 (9)	0.0192 (10)	0.0219 (10)	0.0022 (8)	0.0044 (8)	0.0046 (8)
C25	0.0173 (9)	0.0184 (10)	0.0202 (10)	0.0033 (7)	0.0041 (7)	0.0062 (8)
C26	0.0206 (10)	0.0227 (10)	0.0212 (10)	−0.0013 (8)	0.0037 (8)	0.0040 (8)
C27	0.0207 (10)	0.0209 (10)	0.0185 (9)	0.0029 (8)	0.0032 (8)	0.0046 (8)
C28	0.0204 (10)	0.0179 (10)	0.0187 (9)	0.0010 (8)	0.0048 (8)	0.0048 (7)
C29	0.0196 (9)	0.0198 (10)	0.0165 (9)	0.0024 (8)	0.0037 (7)	0.0034 (7)
C30	0.0211 (10)	0.0214 (10)	0.0168 (9)	0.0015 (8)	0.0029 (7)	0.0047 (8)

C31	0.0308 (12)	0.0282 (12)	0.0183 (10)	−0.0041 (9)	0.0041 (9)	0.0033 (9)
C32	0.0221 (10)	0.0215 (10)	0.0198 (10)	−0.0012 (8)	0.0047 (8)	0.0053 (8)
O4	0.0376 (10)	0.0336 (10)	0.0221 (8)	−0.0068 (8)	0.0012 (7)	0.0128 (7)
C33	0.0257 (11)	0.0278 (11)	0.0181 (10)	−0.0029 (9)	0.0017 (8)	0.0048 (8)
C34	0.0225 (10)	0.0176 (10)	0.0179 (9)	0.0012 (8)	0.0023 (8)	0.0003 (7)
C35	0.0330 (12)	0.0180 (10)	0.0253 (11)	0.0040 (9)	0.0048 (9)	0.0009 (8)
C36	0.0499 (16)	0.0187 (11)	0.0322 (13)	−0.0010 (10)	0.0100 (11)	0.0044 (9)
C37	0.0361 (13)	0.0272 (12)	0.0287 (12)	−0.0128 (10)	0.0099 (10)	−0.0017 (9)
C38	0.0285 (12)	0.0277 (12)	0.0275 (12)	−0.0014 (9)	0.0084 (9)	−0.0042 (9)
C39	0.0249 (11)	0.0213 (11)	0.0250 (11)	0.0041 (8)	0.0034 (9)	−0.0024 (8)
O5	0.0292 (8)	0.0196 (8)	0.0217 (8)	0.0006 (6)	0.0022 (6)	−0.0037 (6)
C40	0.0397 (15)	0.0350 (14)	0.0436 (16)	0.0164 (12)	0.0033 (12)	0.0024 (12)
O6	0.0555 (13)	0.0442 (12)	0.0335 (10)	−0.0245 (10)	0.0172 (10)	−0.0019 (9)
C41	0.0307 (12)	0.0324 (13)	0.0327 (13)	0.0105 (10)	−0.0017 (10)	−0.0003 (10)
C42	0.0389 (14)	0.0220 (12)	0.0368 (14)	0.0067 (10)	0.0038 (11)	−0.0040 (10)
C43	0.0200 (9)	0.0158 (9)	0.0184 (9)	0.0008 (7)	0.0073 (8)	0.0028 (7)
C44	0.0220 (10)	0.0172 (10)	0.0195 (9)	0.0031 (8)	0.0068 (8)	0.0035 (7)
C45	0.0301 (11)	0.0187 (10)	0.0163 (9)	0.0044 (8)	0.0038 (8)	0.0012 (8)
C46	0.0316 (11)	0.0183 (10)	0.0150 (9)	0.0058 (8)	0.0110 (8)	0.0008 (7)
C47	0.0238 (10)	0.0196 (10)	0.0196 (10)	0.0048 (8)	0.0084 (8)	0.0039 (8)
C48	0.0201 (10)	0.0219 (10)	0.0163 (9)	0.0022 (8)	0.0058 (7)	0.0020 (8)
O7	0.0280 (8)	0.0169 (7)	0.0253 (8)	0.0032 (6)	0.0074 (6)	0.0064 (6)
C49	0.0225 (11)	0.0316 (12)	0.0298 (11)	0.0046 (9)	0.0060 (9)	0.0082 (9)
O8	0.0445 (10)	0.0207 (8)	0.0187 (8)	0.0091 (7)	0.0148 (7)	0.0022 (6)
C50	0.0273 (11)	0.0302 (12)	0.0173 (10)	0.0060 (9)	0.0088 (8)	0.0027 (8)
O9	0.0650 (14)	0.0318 (10)	0.0275 (9)	−0.0058 (9)	0.0231 (9)	0.0020 (8)
C51	0.0470 (15)	0.0369 (14)	0.0189 (11)	0.0181 (12)	0.0116 (10)	0.0009 (10)
C52	0.0226 (11)	0.0287 (12)	0.0292 (11)	−0.0025 (9)	0.0072 (9)	−0.0037 (9)
C53	0.0300 (12)	0.0404 (14)	0.0193 (10)	0.0115 (10)	0.0046 (9)	0.0082 (9)
C54	0.0237 (10)	0.0183 (10)	0.0205 (10)	0.0014 (8)	0.0057 (8)	0.0035 (8)
C55	0.0255 (10)	0.0200 (10)	0.0190 (10)	0.0022 (8)	0.0100 (8)	0.0027 (8)
C56	0.0226 (10)	0.0203 (10)	0.0186 (10)	0.0037 (8)	0.0083 (8)	0.0048 (8)
C57	0.0404 (13)	0.0213 (11)	0.0228 (11)	0.0039 (9)	0.0135 (10)	0.0034 (8)
C58	0.0249 (10)	0.0205 (10)	0.0180 (9)	0.0013 (8)	0.0080 (8)	0.0033 (8)
C59	0.0230 (10)	0.0222 (10)	0.0184 (10)	0.0020 (8)	0.0068 (8)	0.0062 (8)
C60	0.0217 (10)	0.0203 (10)	0.0183 (10)	0.0019 (8)	0.0054 (8)	0.0049 (8)
C61	0.0200 (9)	0.0213 (10)	0.0168 (9)	0.0031 (8)	0.0051 (7)	0.0070 (8)
C62	0.0317 (12)	0.0235 (11)	0.0197 (10)	0.0005 (9)	0.0090 (9)	0.0029 (8)
C63	0.0202 (9)	0.0173 (10)	0.0187 (10)	0.0003 (7)	0.0060 (8)	0.0036 (7)
C64	0.0207 (10)	0.0187 (10)	0.0191 (10)	0.0015 (8)	0.0058 (8)	0.0058 (8)
C65	0.0223 (10)	0.0174 (10)	0.0194 (10)	0.0016 (8)	0.0063 (8)	0.0055 (8)
C66	0.0247 (10)	0.0145 (9)	0.0180 (9)	−0.0008 (8)	0.0059 (8)	0.0029 (7)
C67	0.0204 (9)	0.0150 (9)	0.0186 (9)	0.0028 (7)	0.0055 (7)	0.0047 (7)
C68	0.0235 (10)	0.0206 (10)	0.0173 (9)	−0.0013 (8)	0.0057 (8)	0.0013 (8)
C69	0.0215 (10)	0.0150 (9)	0.0189 (9)	−0.0009 (7)	0.0055 (8)	0.0032 (7)
C70	0.0209 (9)	0.0171 (9)	0.0177 (9)	0.0016 (8)	0.0052 (8)	0.0039 (7)
C71	0.0223 (10)	0.0154 (9)	0.0168 (9)	0.0026 (8)	0.0051 (7)	0.0035 (7)
C72	0.0187 (9)	0.0169 (9)	0.0172 (9)	0.0001 (7)	0.0037 (7)	0.0043 (7)

C73	0.0284 (11)	0.0320 (12)	0.0168 (10)	−0.0053 (9)	0.0023 (8)	0.0038 (9)
C74	0.0247 (10)	0.0186 (10)	0.0183 (9)	−0.0003 (8)	0.0043 (8)	0.0048 (8)
O10	0.0391 (10)	0.0304 (9)	0.0194 (8)	−0.0087 (7)	0.0095 (7)	0.0051 (7)
C75	0.0306 (11)	0.0196 (10)	0.0200 (10)	−0.0058 (9)	0.0055 (8)	0.0044 (8)
C76	0.0181 (9)	0.0164 (9)	0.0194 (9)	−0.0018 (7)	0.0020 (7)	0.0035 (7)
C77	0.0216 (10)	0.0263 (12)	0.0296 (12)	0.0051 (9)	0.0029 (9)	0.0007 (9)
C78	0.0206 (11)	0.0378 (14)	0.0401 (14)	−0.0019 (10)	0.0122 (10)	0.0019 (11)
C79	0.0270 (11)	0.0311 (12)	0.0226 (11)	−0.0145 (9)	0.0052 (9)	0.0057 (9)
C80	0.0304 (11)	0.0201 (10)	0.0223 (10)	−0.0050 (8)	−0.0009 (8)	0.0077 (8)
C81	0.0205 (10)	0.0184 (10)	0.0224 (10)	0.0018 (8)	0.0022 (8)	0.0053 (8)
O11	0.0242 (8)	0.0222 (8)	0.0261 (8)	0.0031 (6)	−0.0038 (6)	0.0034 (6)
C82	0.0436 (16)	0.0327 (15)	0.0516 (18)	0.0186 (12)	0.0038 (13)	−0.0017 (12)
O12	0.0517 (13)	0.0497 (13)	0.0286 (9)	−0.0286 (10)	0.0113 (9)	0.0079 (9)
C83	0.0216 (11)	0.0337 (13)	0.0379 (14)	0.0044 (10)	−0.0029 (9)	0.0040 (10)
C84	0.0320 (12)	0.0223 (11)	0.0259 (11)	0.0080 (9)	0.0043 (9)	0.0013 (9)
O13	0.0429 (11)	0.0314 (10)	0.0326 (10)	0.0050 (8)	0.0067 (8)	0.0021 (8)
C85	0.0424 (16)	0.0377 (15)	0.0426 (16)	0.0000 (12)	0.0112 (13)	0.0072 (12)
C86	0.0404 (15)	0.0337 (14)	0.0432 (16)	0.0011 (12)	0.0021 (12)	0.0041 (12)
C87	0.0471 (16)	0.0283 (13)	0.0396 (15)	0.0058 (12)	0.0068 (12)	0.0026 (11)
C88	0.0449 (16)	0.0419 (16)	0.0284 (13)	0.0077 (12)	0.0020 (11)	0.0065 (11)
O14	0.0264 (8)	0.0269 (9)	0.0272 (8)	0.0064 (7)	0.0040 (7)	0.0060 (7)
C89	0.0277 (13)	0.0389 (16)	0.062 (2)	0.0034 (11)	0.0095 (13)	0.0142 (14)
C90	0.0340 (15)	0.0497 (19)	0.056 (2)	0.0115 (13)	0.0037 (13)	0.0094 (15)
C91	0.0371 (14)	0.0363 (14)	0.0253 (12)	0.0054 (11)	0.0027 (10)	0.0042 (10)
C92	0.0393 (15)	0.0414 (15)	0.0368 (14)	0.0092 (12)	0.0165 (12)	0.0059 (11)

Geometric parameters (Å, º)

C1—C12	1.308 (3)	C47—H47A	0.9900
C1—C2	1.539 (3)	C48—C53	1.537 (3)
C1—C6	1.543 (3)	C48—C52	1.547 (3)
C2—O1	1.434 (3)	O7—H95	0.8400
C2—C7	1.526 (3)	C49—H49	0.9800
C2—C3	1.531 (3)	C49—H49A	0.9800
C3—C4	1.519 (3)	C49—H49B	0.9800
C3—H3	0.9900	O8—C50	1.336 (3)
C3—H3A	0.9900	C50—O9	1.208 (3)
C4—O2	1.460 (3)	C50—C51	1.502 (3)
C4—C5	1.513 (3)	C51—H51	0.9800
C4—H4	1.0000	C51—H51A	0.9800
C5—C6	1.545 (3)	C51—H51B	0.9800
C5—H5	0.9900	C52—H52	0.9800
C5—H5A	0.9900	C52—H52A	0.9800
C6—C10	1.533 (3)	C52—H52B	0.9800
C6—C11	1.539 (3)	C53—H53	0.9800
O1—H93	0.8400	C53—H53A	0.9800
C7—H7	0.9800	C53—H53B	0.9800
C7—H7A	0.9800	C54—C55	1.317 (3)

C7—H7B	0.9800	C55—C56	1.470 (3)
O2—C8	1.352 (3)	C55—H55	0.94 (3)
C8—O3	1.199 (3)	C56—C58	1.355 (3)
C8—C9	1.503 (3)	C56—C57	1.499 (3)
C9—H9	0.9800	C57—H57	0.9800
C9—H9A	0.9800	C57—H57A	0.9800
C9—H9B	0.9800	C57—H57B	0.9800
C10—H10	0.9800	C58—C59	1.446 (3)
C10—H10A	0.9800	C58—H58	0.9500
C10—H10B	0.9800	C59—C60	1.355 (3)
C11—H11	0.9800	C59—H59	0.9500
C11—H11A	0.9800	C60—C61	1.451 (3)
C11—H11B	0.9800	C60—H60	0.9500
C12—C13	1.314 (3)	C61—C63	1.366 (3)
C13—C14	1.468 (3)	C61—C62	1.500 (3)
C13—H13	0.99 (3)	C62—H62	0.9800
C14—C16	1.356 (3)	C62—H62A	0.9800
C14—C15	1.503 (3)	C62—H62B	0.9800
C15—H15	0.9800	C63—C64	1.430 (3)
C15—H15A	0.9800	C63—H63	0.9500
C15—H15B	0.9800	C64—C65	1.359 (3)
C16—C17	1.446 (3)	C64—H64	0.9500
C16—H16	0.9500	C65—C66	1.431 (3)
C17—C18	1.355 (3)	C65—H65	0.9500
C17—H17	0.9500	C66—C67	1.362 (3)
C18—C19	1.447 (3)	C66—H66	0.9500
C18—H18	0.9500	C67—C69	1.447 (3)
C19—C21	1.365 (3)	C67—C68	1.500 (3)
C19—C20	1.505 (3)	C68—H68	0.9800
C20—H20	0.9800	C68—H68A	0.9800
C20—H20A	0.9800	C68—H68B	0.9800
C20—H20B	0.9800	C69—C70	1.355 (3)
C21—C22	1.431 (3)	C69—H69	0.9500
C21—H21	0.9500	C70—C71	1.442 (3)
C22—C23	1.360 (3)	C70—H70	0.9500
C22—H22	0.9500	C71—C72	1.355 (3)
C23—C24	1.425 (3)	C71—H71	0.9500
C23—H23	0.9500	C72—C74	1.477 (3)
C24—C25	1.368 (3)	C72—C73	1.507 (3)
C24—H24	0.9500	C73—H73	0.9800
C25—C27	1.443 (3)	C73—H73A	0.9800
C25—C26	1.496 (3)	C73—H73B	0.9800
C26—H26	0.9800	C74—O10	1.219 (3)
C26—H26A	0.9800	C74—C75	1.534 (3)
C26—H26B	0.9800	C75—C76	1.518 (3)
C27—C28	1.357 (3)	C75—H75	0.9900
C27—H27	0.9500	C75—H75A	0.9900
C28—C29	1.444 (3)	C76—O11	1.463 (3)

C28—H28	0.9500	C76—C77	1.477 (3)
C29—C30	1.354 (3)	C76—C81	1.548 (3)
C29—H29	0.9500	C77—O11	1.453 (3)
C30—C32	1.484 (3)	C77—C78	1.513 (4)
C30—C31	1.504 (3)	C77—C82	1.515 (4)
C31—H31	0.9800	C78—C79	1.505 (4)
C31—H31A	0.9800	C78—H78	0.9900
C31—H31B	0.9800	C78—H78A	0.9900
C32—O4	1.222 (3)	C79—O12	1.428 (3)
C32—C33	1.530 (3)	C79—C80	1.521 (4)
C33—C34	1.513 (3)	C79—H79	1.0000
C33—H33	0.9900	C80—C81	1.542 (3)
C33—H33A	0.9900	C80—H80	0.9900
C34—O5	1.461 (3)	C80—H80A	0.9900
C34—C35	1.479 (3)	C81—C83	1.532 (3)
C34—C39	1.552 (3)	C81—C84	1.539 (3)
C35—O5	1.457 (3)	C82—H82	0.9800
C35—C40	1.508 (4)	C82—H82A	0.9800
C35—C36	1.515 (4)	C82—H82B	0.9800
C36—C37	1.518 (4)	O12—H96	0.8400
C36—H36	0.9900	C83—H83	0.9800
C36—H36A	0.9900	C83—H83A	0.9800
C37—O6	1.430 (3)	C83—H83B	0.9800
C37—C38	1.513 (4)	C84—H84	0.9800
C37—H37	1.0000	C84—H84A	0.9800
C38—C39	1.537 (4)	C84—H84B	0.9800
C38—H38	0.9900	O13—C85	1.424 (4)
C38—H38A	0.9900	O13—C87	1.432 (4)
C39—C41	1.539 (3)	C85—C86	1.511 (5)
C39—C42	1.542 (3)	C85—H85	0.9900
C40—H40	0.9800	C85—H85A	0.9900
C40—H40A	0.9800	C86—H86	0.9800
C40—H40B	0.9800	C86—H86A	0.9800
O6—H94	0.8400	C86—H86B	0.9800
C41—H41	0.9800	C87—C88	1.501 (5)
C41—H41A	0.9800	C87—H87	0.9900
C41—H41B	0.9800	C87—H87A	0.9900
C42—H42	0.9800	C88—H88	0.9800
C42—H42A	0.9800	C88—H88A	0.9800
C42—H42B	0.9800	C88—H88B	0.9800
C43—C54	1.300 (3)	O14—C91	1.416 (3)
C43—C44	1.534 (3)	O14—C89	1.443 (3)
C43—C48	1.542 (3)	C89—C90	1.483 (5)
C44—O7	1.431 (3)	C89—H89	0.9900
C44—C49	1.531 (3)	C89—H89A	0.9900
C44—C45	1.541 (3)	C90—H90	0.9800
C45—C46	1.511 (3)	C90—H90A	0.9800
C45—H45	0.9900	C90—H90B	0.9800

C45—H45A	0.9900	C91—C92	1.500 (4)
C46—O8	1.468 (2)	C91—H91	0.9900
C46—C47	1.512 (3)	C91—H91A	0.9900
C46—H46	1.0000	C92—H92	0.9800
C47—C48	1.542 (3)	C92—H92A	0.9800
C47—H47	0.9900	C92—H92B	0.9800
C12—C1—C2	121.40 (19)	C48—C47—H47A	109.1
C12—C1—C6	119.9 (2)	H47—C47—H47A	107.8
C2—C1—C6	118.69 (18)	C53—C48—C47	108.05 (19)
O1—C2—C7	109.74 (19)	C53—C48—C43	110.60 (18)
O1—C2—C3	104.37 (17)	C47—C48—C43	109.20 (17)
C7—C2—C3	110.44 (19)	C53—C48—C52	108.4 (2)
O1—C2—C1	109.83 (18)	C47—C48—C52	110.32 (18)
C7—C2—C1	112.26 (18)	C43—C48—C52	110.26 (19)
C3—C2—C1	109.91 (18)	C44—O7—H95	109.5
C4—C3—C2	111.30 (18)	C44—C49—H49	109.5
C4—C3—H3	109.4	C44—C49—H49A	109.5
C2—C3—H3	109.4	H49—C49—H49A	109.5
C4—C3—H3A	109.4	C44—C49—H49B	109.5
C2—C3—H3A	109.4	H49—C49—H49B	109.5
H3—C3—H3A	108.0	H49A—C49—H49B	109.5
O2—C4—C5	105.19 (17)	C50—O8—C46	118.74 (18)
O2—C4—C3	110.47 (18)	O9—C50—O8	124.1 (2)
C5—C4—C3	110.51 (18)	O9—C50—C51	125.0 (2)
O2—C4—H4	110.2	O8—C50—C51	110.9 (2)
C5—C4—H4	110.2	C50—C51—H51	109.5
C3—C4—H4	110.2	C50—C51—H51A	109.5
C4—C5—C6	113.71 (18)	H51—C51—H51A	109.5
C4—C5—H5	108.8	C50—C51—H51B	109.5
C6—C5—H5	108.8	H51—C51—H51B	109.5
C4—C5—H5A	108.8	H51A—C51—H51B	109.5
C6—C5—H5A	108.8	C48—C52—H52	109.5
H5—C5—H5A	107.7	C48—C52—H52A	109.5
C10—C6—C11	108.56 (19)	H52—C52—H52A	109.5
C10—C6—C1	111.27 (18)	C48—C52—H52B	109.5
C11—C6—C1	110.55 (18)	H52—C52—H52B	109.5
C10—C6—C5	107.64 (18)	H52A—C52—H52B	109.5
C11—C6—C5	110.72 (18)	C48—C53—H53	109.5
C1—C6—C5	108.07 (17)	C48—C53—H53A	109.5
C2—O1—H93	109.5	H53—C53—H53A	109.5
C2—C7—H7	109.5	C48—C53—H53B	109.5
C2—C7—H7A	109.5	H53—C53—H53B	109.5
H7—C7—H7A	109.5	H53A—C53—H53B	109.5
C2—C7—H7B	109.5	C43—C54—C55	178.4 (2)
H7—C7—H7B	109.5	C54—C55—C56	125.0 (2)
H7A—C7—H7B	109.5	C54—C55—H55	124.3 (18)
C8—O2—C4	117.30 (18)	C56—C55—H55	110.7 (18)

O3—C8—O2	124.4 (2)	C58—C56—C55	118.2 (2)
O3—C8—C9	125.0 (2)	C58—C56—C57	124.3 (2)
O2—C8—C9	110.6 (2)	C55—C56—C57	117.42 (19)
C8—C9—H9	109.5	C56—C57—H57	109.5
C8—C9—H9A	109.5	C56—C57—H57A	109.5
H9—C9—H9A	109.5	H57—C57—H57A	109.5
C8—C9—H9B	109.5	C56—C57—H57B	109.5
H9—C9—H9B	109.5	H57—C57—H57B	109.5
H9A—C9—H9B	109.5	H57A—C57—H57B	109.5
C6—C10—H10	109.5	C56—C58—C59	126.6 (2)
C6—C10—H10A	109.5	C56—C58—H58	116.7
H10—C10—H10A	109.5	C59—C58—H58	116.7
C6—C10—H10B	109.5	C60—C59—C58	122.1 (2)
H10—C10—H10B	109.5	C60—C59—H59	119.0
H10A—C10—H10B	109.5	C58—C59—H59	119.0
C6—C11—H11	109.5	C59—C60—C61	125.3 (2)
C6—C11—H11A	109.5	C59—C60—H60	117.3
H11—C11—H11A	109.5	C61—C60—H60	117.3
C6—C11—H11B	109.5	C63—C61—C60	118.6 (2)
H11—C11—H11B	109.5	C63—C61—C62	123.04 (19)
H11A—C11—H11B	109.5	C60—C61—C62	118.29 (19)
C1—C12—C13	177.3 (2)	C61—C62—H62	109.5
C12—C13—C14	125.0 (2)	C61—C62—H62A	109.5
C12—C13—H13	118.1 (18)	H62—C62—H62A	109.5
C14—C13—H13	116.8 (17)	C61—C62—H62B	109.5
C16—C14—C13	118.4 (2)	H62—C62—H62B	109.5
C16—C14—C15	123.8 (2)	H62A—C62—H62B	109.5
C13—C14—C15	117.74 (19)	C61—C63—C64	125.5 (2)
C14—C15—H15	109.5	C61—C63—H63	117.2
C14—C15—H15A	109.5	C64—C63—H63	117.2
H15—C15—H15A	109.5	C65—C64—C63	125.2 (2)
C14—C15—H15B	109.5	C65—C64—H64	117.4
H15—C15—H15B	109.5	C63—C64—H64	117.4
H15A—C15—H15B	109.5	C64—C65—C66	120.1 (2)
C14—C16—C17	126.0 (2)	C64—C65—H65	119.9
C14—C16—H16	117.0	C66—C65—H65	119.9
C17—C16—H16	117.0	C67—C66—C65	129.0 (2)
C18—C17—C16	123.4 (2)	C67—C66—H66	115.5
C18—C17—H17	118.3	C65—C66—H66	115.5
C16—C17—H17	118.3	C66—C67—C69	116.88 (19)
C17—C18—C19	125.1 (2)	C66—C67—C68	123.76 (19)
C17—C18—H18	117.4	C69—C67—C68	119.33 (18)
C19—C18—H18	117.4	C67—C68—H68	109.5
C21—C19—C18	119.0 (2)	C67—C68—H68A	109.5
C21—C19—C20	123.1 (2)	H68—C68—H68A	109.5
C18—C19—C20	117.8 (2)	C67—C68—H68B	109.5
C19—C20—H20	109.5	H68—C68—H68B	109.5
C19—C20—H20A	109.5	H68A—C68—H68B	109.5

H20—C20—H20A	109.5	C70—C69—C67	127.2 (2)
C19—C20—H20B	109.5	C70—C69—H69	116.4
H20—C20—H20B	109.5	C67—C69—H69	116.4
H20A—C20—H20B	109.5	C69—C70—C71	120.68 (19)
C19—C21—C22	125.8 (2)	C69—C70—H70	119.7
C19—C21—H21	117.1	C71—C70—H70	119.7
C22—C21—H21	117.1	C72—C71—C70	126.6 (2)
C23—C22—C21	125.0 (2)	C72—C71—H71	116.7
C23—C22—H22	117.5	C70—C71—H71	116.7
C21—C22—H22	117.5	C71—C72—C74	120.63 (19)
C22—C23—C24	120.4 (2)	C71—C72—C73	123.8 (2)
C22—C23—H23	119.8	C74—C72—C73	115.55 (19)
C24—C23—H23	119.8	C72—C73—H73	109.5
C25—C24—C23	129.0 (2)	C72—C73—H73A	109.5
C25—C24—H24	115.5	H73—C73—H73A	109.5
C23—C24—H24	115.5	C72—C73—H73B	109.5
C24—C25—C27	117.3 (2)	H73—C73—H73B	109.5
C24—C25—C26	123.5 (2)	H73A—C73—H73B	109.5
C27—C25—C26	119.09 (19)	O10—C74—C72	120.2 (2)
C25—C26—H26	109.5	O10—C74—C75	120.1 (2)
C25—C26—H26A	109.5	C72—C74—C75	119.72 (18)
H26—C26—H26A	109.5	C76—C75—C74	110.98 (18)
C25—C26—H26B	109.5	C76—C75—H75	109.4
H26—C26—H26B	109.5	C74—C75—H75	109.4
H26A—C26—H26B	109.5	C76—C75—H75A	109.4
C28—C27—C25	126.8 (2)	C74—C75—H75A	109.4
C28—C27—H27	116.6	H75—C75—H75A	108.0
C25—C27—H27	116.6	O11—C76—C77	59.23 (14)
C27—C28—C29	120.6 (2)	O11—C76—C75	114.03 (18)
C27—C28—H28	119.7	C77—C76—C75	118.0 (2)
C29—C28—H28	119.7	O11—C76—C81	112.28 (17)
C30—C29—C28	126.0 (2)	C77—C76—C81	121.26 (19)
C30—C29—H29	117.0	C75—C76—C81	117.29 (19)
C28—C29—H29	117.0	O11—C77—C76	59.93 (14)
C29—C30—C32	119.7 (2)	O11—C77—C78	115.6 (2)
C29—C30—C31	124.6 (2)	C76—C77—C78	119.8 (2)
C32—C30—C31	115.66 (19)	O11—C77—C82	114.2 (2)
C30—C31—H31	109.5	C76—C77—C82	122.3 (2)
C30—C31—H31A	109.5	C78—C77—C82	113.4 (2)
H31—C31—H31A	109.5	C79—C78—C77	113.7 (2)
C30—C31—H31B	109.5	C79—C78—H78	108.8
H31—C31—H31B	109.5	C77—C78—H78	108.8
H31A—C31—H31B	109.5	C79—C78—H78A	108.8
O4—C32—C30	120.2 (2)	C77—C78—H78A	108.8
O4—C32—C33	119.6 (2)	H78—C78—H78A	107.7
C30—C32—C33	120.25 (19)	O12—C79—C78	110.8 (2)
C34—C33—C32	111.39 (18)	O12—C79—C80	112.9 (2)
C34—C33—H33	109.4	C78—C79—C80	109.50 (19)

C32—C33—H33	109.4	O12—C79—H79	107.8
C34—C33—H33A	109.4	C78—C79—H79	107.8
C32—C33—H33A	109.4	C80—C79—H79	107.8
H33—C33—H33A	108.0	C79—C80—C81	113.24 (19)
O5—C34—C35	59.40 (14)	C79—C80—H80	108.9
O5—C34—C33	114.21 (18)	C81—C80—H80	108.9
C35—C34—C33	118.6 (2)	C79—C80—H80A	108.9
O5—C34—C39	112.22 (18)	C81—C80—H80A	108.9
C35—C34—C39	121.4 (2)	H80—C80—H80A	107.7
C33—C34—C39	116.5 (2)	C83—C81—C84	106.6 (2)
O5—C35—C34	59.70 (14)	C83—C81—C80	107.16 (19)
O5—C35—C40	113.8 (2)	C84—C81—C80	110.80 (19)
C34—C35—C40	123.2 (2)	C83—C81—C76	112.50 (19)
O5—C35—C36	115.1 (2)	C84—C81—C76	108.33 (18)
C34—C35—C36	119.6 (2)	C80—C81—C76	111.35 (19)
C40—C35—C36	113.4 (2)	C77—O11—C76	60.85 (14)
C35—C36—C37	114.2 (2)	C77—C82—H82	109.5
C35—C36—H36	108.7	C77—C82—H82A	109.5
C37—C36—H36	108.7	H82—C82—H82A	109.5
C35—C36—H36A	108.7	C77—C82—H82B	109.5
C37—C36—H36A	108.7	H82—C82—H82B	109.5
H36—C36—H36A	107.6	H82A—C82—H82B	109.5
O6—C37—C38	112.0 (2)	C79—O12—H96	109.5
O6—C37—C36	110.7 (3)	C81—C83—H83	109.5
C38—C37—C36	109.9 (2)	C81—C83—H83A	109.5
O6—C37—H37	108.0	H83—C83—H83A	109.5
C38—C37—H37	108.0	C81—C83—H83B	109.5
C36—C37—H37	108.0	H83—C83—H83B	109.5
C37—C38—C39	114.0 (2)	H83A—C83—H83B	109.5
C37—C38—H38	108.7	C81—C84—H84	109.5
C39—C38—H38	108.7	C81—C84—H84A	109.5
C37—C38—H38A	108.7	H84—C84—H84A	109.5
C39—C38—H38A	108.7	C81—C84—H84B	109.5
H38—C38—H38A	107.6	H84—C84—H84B	109.5
C38—C39—C41	110.9 (2)	H84A—C84—H84B	109.5
C38—C39—C42	106.2 (2)	C85—O13—C87	113.5 (2)
C41—C39—C42	107.7 (2)	O13—C85—C86	114.5 (3)
C38—C39—C34	111.5 (2)	O13—C85—H85	108.6
C41—C39—C34	107.98 (19)	C86—C85—H85	108.6
C42—C39—C34	112.5 (2)	O13—C85—H85A	108.6
C35—O5—C34	60.90 (14)	C86—C85—H85A	108.6
C35—C40—H40	109.5	H85—C85—H85A	107.6
C35—C40—H40A	109.5	C85—C86—H86	109.5
H40—C40—H40A	109.5	C85—C86—H86A	109.5
C35—C40—H40B	109.5	H86—C86—H86A	109.5
H40—C40—H40B	109.5	C85—C86—H86B	109.5
H40A—C40—H40B	109.5	H86—C86—H86B	109.5
C37—O6—H94	109.5	H86A—C86—H86B	109.5

C39—C41—H41	109.5	O13—C87—C88	108.6 (2)
C39—C41—H41A	109.5	O13—C87—H87	110.0
H41—C41—H41A	109.5	C88—C87—H87	110.0
C39—C41—H41B	109.5	O13—C87—H87A	110.0
H41—C41—H41B	109.5	C88—C87—H87A	110.0
H41A—C41—H41B	109.5	H87—C87—H87A	108.4
C39—C42—H42	109.5	C87—C88—H88	109.5
C39—C42—H42A	109.5	C87—C88—H88A	109.5
H42—C42—H42A	109.5	H88—C88—H88A	109.5
C39—C42—H42B	109.5	C87—C88—H88B	109.5
H42—C42—H42B	109.5	H88—C88—H88B	109.5
H42A—C42—H42B	109.5	H88A—C88—H88B	109.5
C54—C43—C44	120.2 (2)	C91—O14—C89	113.0 (2)
C54—C43—C48	120.9 (2)	O14—C89—C90	114.5 (3)
C44—C43—C48	118.75 (17)	O14—C89—H89	108.6
O7—C44—C49	110.42 (18)	C90—C89—H89	108.6
O7—C44—C43	106.09 (17)	O14—C89—H89A	108.6
C49—C44—C43	111.84 (18)	C90—C89—H89A	108.6
O7—C44—C45	109.56 (17)	H89—C89—H89A	107.6
C49—C44—C45	108.72 (19)	C89—C90—H90	109.5
C43—C44—C45	110.19 (17)	C89—C90—H90A	109.5
C46—C45—C44	112.12 (18)	H90—C90—H90A	109.5
C46—C45—H45	109.2	C89—C90—H90B	109.5
C44—C45—H45	109.2	H90—C90—H90B	109.5
C46—C45—H45A	109.2	H90A—C90—H90B	109.5
C44—C45—H45A	109.2	O14—C91—C92	108.3 (2)
H45—C45—H45A	107.9	O14—C91—H91	110.0
O8—C46—C45	107.48 (18)	C92—C91—H91	110.0
O8—C46—C47	106.00 (17)	O14—C91—H91A	110.0
C45—C46—C47	110.93 (17)	C92—C91—H91A	110.0
O8—C46—H46	110.8	H91—C91—H91A	108.4
C45—C46—H46	110.8	C91—C92—H92	109.5
C47—C46—H46	110.8	C91—C92—H92A	109.5
C46—C47—C48	112.64 (18)	H92—C92—H92A	109.5
C46—C47—H47	109.1	C91—C92—H92B	109.5
C48—C47—H47	109.1	H92—C92—H92B	109.5
C46—C47—H47A	109.1	H92A—C92—H92B	109.5

C12—C1—C2—O1	−112.5 (2)	C54—C43—C44—C49	17.8 (3)
C6—C1—C2—O1	66.7 (2)	C48—C43—C44—C49	−165.78 (19)
C12—C1—C2—C7	9.9 (3)	C54—C43—C44—C45	138.8 (2)
C6—C1—C2—C7	−170.9 (2)	C48—C43—C44—C45	−44.7 (2)
C12—C1—C2—C3	133.2 (2)	O7—C44—C45—C46	−66.2 (2)
C6—C1—C2—C3	−47.6 (3)	C49—C44—C45—C46	173.10 (19)
O1—C2—C3—C4	−65.2 (2)	C43—C44—C45—C46	50.2 (2)
C7—C2—C3—C4	176.89 (19)	C44—C45—C46—O8	−175.00 (17)
C1—C2—C3—C4	52.5 (2)	C44—C45—C46—C47	−59.5 (2)
C2—C3—C4—O2	−176.13 (17)	O8—C46—C47—C48	176.65 (17)

C2—C3—C4—C5	−60.1 (2)	C45—C46—C47—C48	60.3 (2)
O2—C4—C5—C6	179.23 (18)	C46—C47—C48—C53	−171.05 (19)
C3—C4—C5—C6	60.0 (2)	C46—C47—C48—C43	−50.7 (2)
C12—C1—C6—C10	−17.4 (3)	C46—C47—C48—C52	70.6 (2)
C2—C1—C6—C10	163.40 (19)	C54—C43—C48—C53	−20.1 (3)
C12—C1—C6—C11	103.3 (2)	C44—C43—C48—C53	163.46 (19)
C2—C1—C6—C11	−75.9 (2)	C54—C43—C48—C47	−138.9 (2)
C12—C1—C6—C5	−135.4 (2)	C44—C43—C48—C47	44.7 (2)
C2—C1—C6—C5	45.4 (2)	C54—C43—C48—C52	99.7 (2)
C4—C5—C6—C10	−170.57 (19)	C44—C43—C48—C52	−76.7 (2)
C4—C5—C6—C11	70.9 (2)	C45—C46—O8—C50	−100.1 (2)
C4—C5—C6—C1	−50.3 (2)	C47—C46—O8—C50	141.2 (2)
C5—C4—O2—C8	154.8 (2)	C46—O8—C50—O9	−2.1 (4)
C3—C4—O2—C8	−86.0 (2)	C46—O8—C50—C51	176.1 (2)
C4—O2—C8—O3	8.8 (4)	C54—C55—C56—C58	−171.5 (2)
C4—O2—C8—C9	−170.9 (2)	C54—C55—C56—C57	8.1 (4)
C12—C13—C14—C16	177.9 (2)	C55—C56—C58—C59	176.8 (2)
C12—C13—C14—C15	−2.9 (3)	C57—C56—C58—C59	−2.8 (4)
C13—C14—C16—C17	−179.3 (2)	C56—C58—C59—C60	−175.3 (2)
C15—C14—C16—C17	1.5 (4)	C58—C59—C60—C61	177.5 (2)
C14—C16—C17—C18	172.2 (2)	C59—C60—C61—C63	−179.8 (2)
C16—C17—C18—C19	−177.0 (2)	C59—C60—C61—C62	−2.5 (3)
C17—C18—C19—C21	176.5 (2)	C60—C61—C63—C64	−177.6 (2)
C17—C18—C19—C20	−1.6 (3)	C62—C61—C63—C64	5.2 (4)
C18—C19—C21—C22	−179.3 (2)	C61—C63—C64—C65	−173.2 (2)
C20—C19—C21—C22	−1.2 (4)	C63—C64—C65—C66	−175.7 (2)
C19—C21—C22—C23	175.0 (2)	C64—C65—C66—C67	−179.3 (2)
C21—C22—C23—C24	177.6 (2)	C65—C66—C67—C69	−175.5 (2)
C22—C23—C24—C25	−175.6 (2)	C65—C66—C67—C68	2.7 (4)
C23—C24—C25—C27	174.5 (2)	C66—C67—C69—C70	−176.3 (2)
C23—C24—C25—C26	−3.1 (4)	C68—C67—C69—C70	5.5 (3)
C24—C25—C27—C28	−178.9 (2)	C67—C69—C70—C71	−177.1 (2)
C26—C25—C27—C28	−1.2 (3)	C69—C70—C71—C72	−175.4 (2)
C25—C27—C28—C29	176.7 (2)	C70—C71—C72—C74	−177.2 (2)
C27—C28—C29—C30	169.3 (2)	C70—C71—C72—C73	2.6 (4)
C28—C29—C30—C32	−179.4 (2)	C71—C72—C74—O10	175.5 (2)
C28—C29—C30—C31	−2.5 (4)	C73—C72—C74—O10	−4.3 (3)
C29—C30—C32—O4	167.6 (2)	C71—C72—C74—C75	−4.4 (3)
C31—C30—C32—O4	−9.6 (3)	C73—C72—C74—C75	175.8 (2)
C29—C30—C32—C33	−13.5 (3)	O10—C74—C75—C76	1.1 (3)
C31—C30—C32—C33	169.3 (2)	C72—C74—C75—C76	−179.1 (2)
O4—C32—C33—C34	15.5 (3)	C74—C75—C76—O11	−137.9 (2)
C30—C32—C33—C34	−163.4 (2)	C74—C75—C76—C77	−71.3 (3)
C32—C33—C34—O5	−144.8 (2)	C74—C75—C76—C81	87.9 (2)
C32—C33—C34—C35	−77.8 (3)	C75—C76—C77—O11	−102.7 (2)
C32—C33—C34—C39	81.7 (3)	C81—C76—C77—O11	98.9 (2)
C33—C34—C35—O5	−102.7 (2)	O11—C76—C77—C78	−104.1 (2)
C39—C34—C35—O5	98.8 (2)	C75—C76—C77—C78	153.2 (2)

O5—C34—C35—C40	100.1 (3)	C81—C76—C77—C78	−5.2 (3)
C33—C34—C35—C40	−2.6 (3)	O11—C76—C77—C82	101.2 (3)
C39—C34—C35—C40	−161.0 (2)	C75—C76—C77—C82	−1.6 (3)
O5—C34—C35—C36	−103.5 (2)	C81—C76—C77—C82	−159.9 (2)
C33—C34—C35—C36	153.8 (2)	O11—C77—C78—C79	−44.4 (3)
C39—C34—C35—C36	−4.7 (3)	C76—C77—C78—C79	24.2 (3)
O5—C35—C36—C37	−45.3 (3)	C82—C77—C78—C79	−178.9 (2)
C34—C35—C36—C37	22.7 (3)	C77—C78—C79—O12	−177.5 (2)
C40—C35—C36—C37	−178.7 (2)	C77—C78—C79—C80	−52.4 (3)
C35—C36—C37—O6	−174.7 (2)	O12—C79—C80—C81	−171.5 (2)
C35—C36—C37—C38	−50.4 (3)	C78—C79—C80—C81	64.5 (3)
O6—C37—C38—C39	−173.6 (2)	C79—C80—C81—C83	−167.5 (2)
C36—C37—C38—C39	62.9 (3)	C79—C80—C81—C84	76.5 (3)
C37—C38—C39—C41	76.7 (3)	C79—C80—C81—C76	−44.1 (3)
C37—C38—C39—C42	−166.5 (2)	O11—C76—C81—C83	−158.4 (2)
C37—C38—C39—C34	−43.7 (3)	C77—C76—C81—C83	135.0 (2)
O5—C34—C39—C38	81.3 (2)	C75—C76—C81—C83	−23.5 (3)
C35—C34—C39—C38	14.5 (3)	O11—C76—C81—C84	−40.8 (2)
C33—C34—C39—C38	−144.4 (2)	C77—C76—C81—C84	−107.3 (2)
O5—C34—C39—C41	−40.8 (3)	C75—C76—C81—C84	94.2 (2)
C35—C34—C39—C41	−107.6 (3)	O11—C76—C81—C80	81.3 (2)
C33—C34—C39—C41	93.5 (2)	C77—C76—C81—C80	14.7 (3)
O5—C34—C39—C42	−159.5 (2)	C75—C76—C81—C80	−143.77 (19)
C35—C34—C39—C42	133.7 (2)	C78—C77—O11—C76	111.1 (2)
C33—C34—C39—C42	−25.2 (3)	C82—C77—O11—C76	−114.6 (2)
C40—C35—O5—C34	−115.8 (2)	C75—C76—O11—C77	109.4 (2)
C36—C35—O5—C34	111.0 (2)	C81—C76—O11—C77	−114.1 (2)
C33—C34—O5—C35	110.2 (2)	C87—O13—C85—C86	69.4 (3)
C39—C34—O5—C35	−114.4 (2)	C85—O13—C87—C88	−176.9 (2)
C54—C43—C44—O7	−102.7 (2)	C91—O14—C89—C90	71.2 (3)
C48—C43—C44—O7	73.8 (2)	C89—O14—C91—C92	−176.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H93···O14^{i}	0.84	2.13	2.898 (2)	153
O6—H94···O13^{ii}	0.84	2.07	2.907 (3)	174
O7—H95···O14^{iii}	0.84	2.06	2.899 (2)	173
O12—H96···O9^{iv}	0.84	2.20	2.945 (3)	147
C91—H91*A*···O10^{ii}	0.99	2.60	3.589 (3)	173

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