# organic compounds

# (E)-3-(4-Cyclohexyl-3-fluorobenzyl-idene)chroman-4-one

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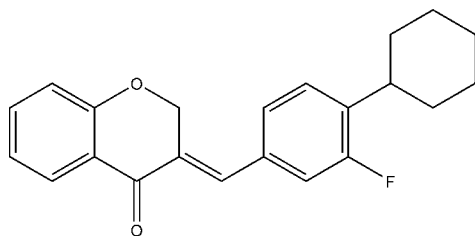Correspondence e-mail: koorbanally@ukzn.ac.za

The title compound, $C_{22}H_{21}FO_2$, exhibits substitutional disorder of the F atom and a H atom in the asymmetric unit with different occupancies, the refined F:H ratio being 0.80 (2):0.20 (2). The dihedral angle between the fluorinated benzene ring and the benzene ring of the chromanone system is 37.30°. There are two relatively high residual electron-density peaks associated with the disorder.

## Related literature

For the preparation, see: Shaikh *et al.* (2011). For related structures, see: Gopaul *et al.* (2012); Marx *et al.* (2008); Suresh *et al.* (2007). For the biological activity of this class of compound, see: du Toit *et al.* (2010). This compound may undergo chemical conversion into the (*E*)- and (*Z*)-isomers, see: Kirkiacharian *et al.* (1984).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{22}H_{21}FO_2$ | $M_r = 336.39$ |
| Triclinic, $P\bar{1}$ | $V = 824.45$ (3) Å$^3$ |
| $a = 6.8351$ (1) Å | $Z = 2$ |
| $b = 8.1483$ (2) Å | Mo $K\alpha$ radiation |
| $c = 15.7931$ (3) Å | $\mu = 0.09$ mm$^{-1}$ |
| $\alpha = 76.661$ (1)° | $T = 446$ K |
| $\beta = 81.769$ (1)° | $0.34 \times 0.33 \times 0.19$ mm |
| $\gamma = 75.287$ (1)° | |

### Data collection

| | |
|---|---|
| Bruker SMART APEXII CCD diffractometer | 18883 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2008) | 4104 independent reflections |
| $T_{min} = 0.969$, $T_{max} = 0.983$ | 3637 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.029$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.058$ | 21 restraints |
| $wR(F^2) = 0.173$ | H-atom parameters constrained |
| $S = 1.05$ | $\Delta\rho_{max} = 0.96$ e Å$^{-3}$ |
| 4104 reflections | $\Delta\rho_{min} = -1.05$ e Å$^{-3}$ |
| 233 parameters | |

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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# supplementary materials

# (*E*)-3-(4-Cyclohexyl-3-fluorobenzylidene)chroman-4-one

## Kaalin Gopaul, Mahidansha M. Shaikh, Neil A. Koorbanally, Deresh Ramjugernath and Bernard Omondi

**Comment**

The title compound, 3-(4-cyclohexyl-3-fluorobenzylidene)chroman-4-one, belongs to the homoisoflavonoid class of compounds, which are *α,β* unsaturated carbonyl compounds containing two aromatic rings. They are a group of naturally occurring molecules that are structurally related to isoflavonoids but differ by containing one more carbon atoms (Kirkiacharian *et al.*, 1984). This compound may undergo chemical conversion into the (E)- and (*Z*)-isomers (Kirkiacharian *et al.*, 1984). The 3-benzylidene-4-chromanones have been shown to display a wide range of biological activities (du Toit *et al.*, 2010). The most commonly used procedure for the synthesis of homoisoflavonoids involves the condensation of chroman-4-one with an aromatic aldehyde in the presence of an acidic or basic catalyst (Shaikh *et al.*, 2011). We have recently been involved in the synthesis and characterization of fluorinated homoisoflavonoids in the search for lead pharmaceuticals (Gopaul *et al.*, 2012).

In the molecular structure, the dihedral angle between the fluorinated benzene moiety and the benzene ring of the chromanone moiety is 37.30°. The cyclohexane moiety on the fluorinated benzene ring is attached to the least sterically hindered *para*-position of the phenyl ring and adopts a chair confirmation.

**Experimental**

A mixture of chroman-4-one (1.00 g, 6.749 mmol), 3,4-difluorobenzaldehyde (1.15 g, 8.099 mmol) and 10–15 drops of piperidine in cyclohexane was heated at 80°C for 24 hrs. The reaction mixture was monitored for completion by thin layer chromatography. Upon completion, the reaction mixture was cooled, diluted with water and neutralized using 10% HCl. The reaction mixture was extracted with ethyl acetate (3 × 30 ml). The ethyl acetate layers were combined, washed with brine (20 ml), water (2 × 10 ml) and dried over anhydrous magnesium sulfate. The solvent was reduced and the compound purified by column chromatography using silica gel (Merck 9385, 40–63 $\mu$m particle size) with a mobile phase of 2% ethyl acetate in hexane to yield the title compound.

^{1}H NMR: $\delta$ (p.p.m.): 1.65 (7*H*, m, H-5″- H-11″), 3.12 (4*H*, m, H-1″- H-4″), 5.36 (2*H*, d, *J*=1.68 Hz, H-2), 7.06–6.92 (5*H*, m, H-2′, H-5′, H-6′, H-6, H-8), 7.46 (1*H*, ddd, *J*=8.48, 6.96, 1.52 Hz, H-7), 7.74 (1*H*, s, H-9), 8.00 (1*H*, dd, *J*=7.84, 1.44 Hz, H-5). ^{13}C NMR: $\delta$ (p.p.m.): 181.9, 160.9, 154.7 (*J*=246.6 Hz), 142.3 (*J*=8.24 Hz), 136.4 (*J*=1.94 Hz), 135.70, 129.2, 127.9, 127.3 (*J*=2.71 Hz), 122.1, 121.9, 118.7 (*J*=3.94 Hz), 117.83, 117.79 (*J*=22.02 Hz), 67.7, 51.5 (*J*=4.19 Hz), 25.9, 24.2.

**Computing details**

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare

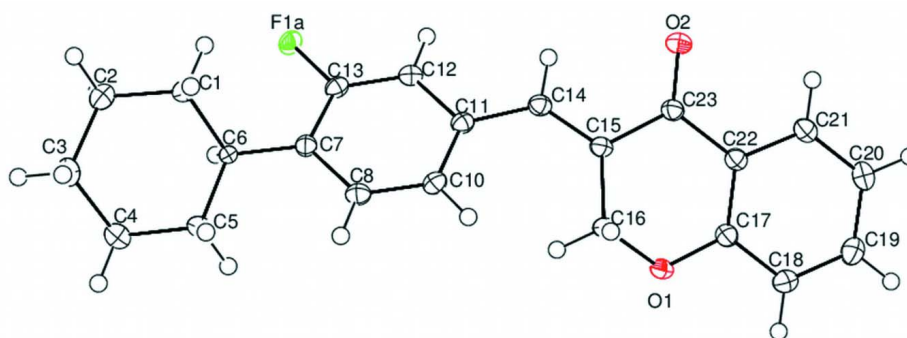material for publication: *WinGX* (Farrugia, 1999).



**Figure 1**

The asymmetric unit of the title compound with displacement ellipsoids drawn at the 50% probability level. The atoms F1a/F1b and H-8/H-13 are disordered and only F1a and H-8 are shown.

**(*E*)-3-(4-Cyclohexyl-3-fluorobenzylidene)chroman-4-one**

*Crystal data*

| | |
|---|---|
| $C_{22}H_{21}FO_2$ | $Z = 2$ |
| $M_r = 336.39$ | $F(000) = 356$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.355$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 6.8351$ (1) Å | Cell parameters from 18935 reflections |
| $b = 8.1483$ (2) Å | $\theta = 2.6–28.5°$ |
| $c = 15.7931$ (3) Å | $\mu = 0.09$ mm$^{-1}$ |
| $\alpha = 76.661$ (1)° | $T = 446$ K |
| $\beta = 81.769$ (1)° | Block, yellow |
| $\gamma = 75.287$ (1)° | $0.34 \times 0.33 \times 0.19$ mm |
| $V = 824.45$ (3) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD diffractometer | 4104 independent reflections |
| Graphite monochromator | 3637 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int} = 0.029$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2008) | $\theta_{max} = 28.5°$, $\theta_{min} = 2.6°$ |
| $T_{min} = 0.969$, $T_{max} = 0.983$ | $h = -9\rightarrow9$ |
| 18883 measured reflections | $k = -8\rightarrow10$ |
| | $l = -21\rightarrow21$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.058$ | |
| $wR(F^2) = 0.173$ | H-atom parameters constrained |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0944P)^2 + 0.7446P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 4104 reflections | |
| 233 parameters | $(\Delta/\sigma)_{max} < 0.001$ |
| 21 restraints | $\Delta\rho_{max} = 0.96$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{min} = -1.05$ e Å$^{-3}$ |

*Special details*

**Experimental**. Carbon-bound H-atoms were placed in calculated positions [C—H = 0.97 Å for Methylene H atoms, 0.98 Å for methine and 0.93 Å for aromatic H atoms; $U_{iso}$(H) = 1.2$U_{eq}$(C)] and were included in the refinement in the riding model approximation. Disorder: Disorder was found for the F– and H-atoms, which is not an uncommon situation. The disorder was modelled for F– and H– atoms (80:30) using PART instructions and the total occupancy at each atom site was kept as 1 during the refinement by means of a SUMFIX constraint. The F-atoms involved in disorder were modelled with anisotropic thermal parameters.

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å$^2$)*

|  | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.2972 (3) | 0.3337 (3) | 0.18026 (11) | 0.0240 (4) | |
| H1A | 0.4375 | 0.2691 | 0.1775 | 0.029* | |
| H1B | 0.297 | 0.4558 | 0.1702 | 0.029* | |
| C2 | 0.1930 (3) | 0.3034 (3) | 0.10912 (11) | 0.0256 (4) | |
| H2A | 0.215 | 0.1798 | 0.1126 | 0.031* | |
| H2B | 0.2531 | 0.3532 | 0.0527 | 0.031* | |
| C3 | −0.0336 (3) | 0.3826 (3) | 0.11618 (12) | 0.0269 (4) | |
| H3A | −0.0566 | 0.5079 | 0.1001 | 0.032* | |
| H3B | −0.0978 | 0.3443 | 0.0757 | 0.032* | |
| C4 | −0.1284 (3) | 0.3313 (3) | 0.20779 (12) | 0.0276 (4) | |
| H4A | −0.129 | 0.2093 | 0.2193 | 0.033* | |
| H4B | −0.2683 | 0.3964 | 0.2122 | 0.033* | |
| C5 | −0.0171 (2) | 0.3636 (3) | 0.27620 (11) | 0.0252 (4) | |
| H5A | −0.0337 | 0.4874 | 0.2704 | 0.03* | |
| H5B | −0.0759 | 0.3186 | 0.3338 | 0.03* | |
| C6 | 0.1987 (2) | 0.28131 (19) | 0.26771 (9) | 0.0131 (3) | |
| H6 | 0.1978 | 0.1604 | 0.2696 | 0.016* | |
| C7 | 0.3101 (2) | 0.2672 (2) | 0.33810 (10) | 0.0158 (3) | |
| C8 | 0.2403 (2) | 0.3561 (2) | 0.40676 (10) | 0.0181 (3) | |
| H8 | 0.1123 | 0.4306 | 0.4063 | 0.022* | 0.803 (4) |
| F1B | 0.0633 (2) | 0.4701 (2) | 0.41034 (10) | 0.0309 (17) | 0.197 (4) |
| C10 | 0.3560 (2) | 0.3365 (2) | 0.47542 (10) | 0.0178 (3) | |
| H10 | 0.3038 | 0.3982 | 0.5195 | 0.021* | |
| C11 | 0.5499 (2) | 0.22563 (19) | 0.47953 (10) | 0.0160 (3) | |
| C12 | 0.6215 (2) | 0.13448 (19) | 0.41124 (10) | 0.0164 (3) | |
| H12 | 0.7496 | 0.0599 | 0.4114 | 0.02* | |
| C13 | 0.5036 (2) | 0.15504 (19) | 0.34448 (10) | 0.0161 (3) | |
| H13 | 0.5545 | 0.0913 | 0.3011 | 0.019* | 0.197 (4) |
| F1A | 0.57542 (18) | 0.05863 (15) | 0.28206 (8) | 0.0190 (4) | 0.803 (4) |
| C14 | 0.6861 (2) | 0.1993 (2) | 0.54697 (10) | 0.0170 (3) | |
| H14 | 0.8215 | 0.1522 | 0.5311 | 0.02* | |

| | | | |
|---|---|---|---|
| C15 | 0.6495 (2) | 0.23152 (19) | 0.62847 (10) | 0.0159 (3) |
| C16 | 0.4451 (2) | 0.3066 (2) | 0.67092 (10) | 0.0183 (3) |
| H16A | 0.4237 | 0.4318 | 0.6582 | 0.022* |
| H16B | 0.3413 | 0.2779 | 0.6448 | 0.022* |
| C17 | 0.5798 (2) | 0.2205 (2) | 0.81068 (10) | 0.0180 (3) |
| C18 | 0.5371 (3) | 0.2086 (2) | 0.90100 (11) | 0.0231 (3) |
| H18 | 0.404 | 0.2192 | 0.9261 | 0.028* |
| C19 | 0.6940 (3) | 0.1809 (2) | 0.95265 (11) | 0.0239 (4) |
| H19 | 0.6657 | 0.1728 | 1.0127 | 0.029* |
| C20 | 0.8948 (3) | 0.1650 (2) | 0.91576 (11) | 0.0223 (3) |
| H20 | 0.9991 | 0.1495 | 0.9508 | 0.027* |
| C21 | 0.9374 (2) | 0.1725 (2) | 0.82692 (11) | 0.0196 (3) |
| H21 | 1.0712 | 0.159 | 0.8025 | 0.023* |
| C22 | 0.7803 (2) | 0.20013 (19) | 0.77313 (10) | 0.0165 (3) |
| C23 | 0.8274 (2) | 0.1979 (2) | 0.67917 (10) | 0.0180 (3) |
| O1 | 0.41878 (17) | 0.24763 (18) | 0.76439 (8) | 0.0230 (3) |
| O2 | 1.00278 (19) | 0.1688 (2) | 0.64622 (9) | 0.0303 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0204 (8) | 0.0353 (9) | 0.0172 (7) | −0.0094 (7) | 0.0026 (6) | −0.0064 (6) |
| C2 | 0.0245 (8) | 0.0333 (9) | 0.0185 (8) | −0.0042 (7) | −0.0007 (6) | −0.0081 (7) |
| C3 | 0.0239 (8) | 0.0373 (10) | 0.0222 (8) | −0.0083 (7) | −0.0058 (6) | −0.0078 (7) |
| C4 | 0.0189 (8) | 0.0393 (10) | 0.0255 (9) | −0.0077 (7) | −0.0028 (6) | −0.0070 (7) |
| C5 | 0.0147 (7) | 0.0397 (10) | 0.0221 (8) | −0.0066 (6) | 0.0001 (6) | −0.0085 (7) |
| C6 | 0.0111 (6) | 0.0177 (7) | 0.0106 (6) | −0.0035 (5) | −0.0004 (5) | −0.0031 (5) |
| C7 | 0.0165 (7) | 0.0173 (7) | 0.0144 (6) | −0.0067 (5) | −0.0008 (5) | −0.0020 (5) |
| C8 | 0.0161 (7) | 0.0170 (7) | 0.0197 (7) | −0.0019 (5) | 0.0003 (5) | −0.0042 (6) |
| F1B | 0.023 (3) | 0.034 (3) | 0.032 (3) | 0.009 (2) | −0.007 (2) | −0.014 (2) |
| C10 | 0.0189 (7) | 0.0172 (7) | 0.0166 (7) | −0.0026 (6) | 0.0006 (5) | −0.0053 (5) |
| C11 | 0.0168 (7) | 0.0154 (7) | 0.0160 (7) | −0.0054 (5) | 0.0006 (5) | −0.0029 (5) |
| C12 | 0.0154 (7) | 0.0151 (7) | 0.0181 (7) | −0.0034 (5) | 0.0007 (5) | −0.0034 (5) |
| C13 | 0.0188 (7) | 0.0143 (7) | 0.0158 (7) | −0.0049 (5) | 0.0017 (5) | −0.0047 (5) |
| F1A | 0.0210 (6) | 0.0186 (6) | 0.0182 (6) | −0.0015 (4) | −0.0006 (4) | −0.0093 (4) |
| C14 | 0.0151 (7) | 0.0161 (7) | 0.0194 (7) | −0.0024 (5) | −0.0004 (5) | −0.0051 (5) |
| C15 | 0.0133 (6) | 0.0159 (7) | 0.0184 (7) | −0.0031 (5) | −0.0001 (5) | −0.0045 (5) |
| C16 | 0.0137 (7) | 0.0242 (8) | 0.0158 (7) | −0.0025 (6) | 0.0006 (5) | −0.0047 (6) |
| C17 | 0.0168 (7) | 0.0190 (7) | 0.0189 (7) | −0.0044 (5) | −0.0020 (6) | −0.0046 (6) |
| C18 | 0.0197 (7) | 0.0292 (9) | 0.0197 (8) | −0.0053 (6) | 0.0010 (6) | −0.0057 (6) |
| C19 | 0.0283 (9) | 0.0262 (8) | 0.0180 (7) | −0.0070 (7) | −0.0029 (6) | −0.0046 (6) |
| C20 | 0.0240 (8) | 0.0218 (8) | 0.0232 (8) | −0.0064 (6) | −0.0082 (6) | −0.0037 (6) |
| C21 | 0.0172 (7) | 0.0192 (7) | 0.0234 (8) | −0.0046 (6) | −0.0035 (6) | −0.0050 (6) |
| C22 | 0.0155 (7) | 0.0153 (7) | 0.0190 (7) | −0.0029 (5) | −0.0020 (5) | −0.0043 (5) |
| C23 | 0.0142 (7) | 0.0199 (7) | 0.0205 (7) | −0.0025 (5) | −0.0007 (5) | −0.0076 (6) |
| O1 | 0.0133 (5) | 0.0381 (7) | 0.0171 (6) | −0.0064 (5) | 0.0002 (4) | −0.0048 (5) |
| O2 | 0.0140 (6) | 0.0507 (9) | 0.0273 (7) | −0.0028 (5) | 0.0010 (5) | −0.0172 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.467 (2) | C11—C14 | 1.457 (2) |
| C1—C2 | 1.509 (2) | C12—C13 | 1.372 (2) |
| C1—H1A | 0.97 | C12—H12 | 0.93 |
| C1—H1B | 0.97 | C13—F1A | 1.3611 (18) |
| C2—C3 | 1.518 (2) | C13—H13 | 0.93 |
| C2—H2A | 0.97 | C14—C15 | 1.349 (2) |
| C2—H2B | 0.97 | C14—H14 | 0.93 |
| C3—C4 | 1.509 (3) | C15—C23 | 1.484 (2) |
| C3—H3A | 0.97 | C15—C16 | 1.504 (2) |
| C3—H3B | 0.97 | C16—O1 | 1.4433 (19) |
| C4—C5 | 1.511 (2) | C16—H16A | 0.97 |
| C4—H4A | 0.97 | C16—H16B | 0.97 |
| C4—H4B | 0.97 | C17—O1 | 1.3517 (19) |
| C5—C6 | 1.458 (2) | C17—C22 | 1.398 (2) |
| C5—H5A | 0.97 | C17—C18 | 1.400 (2) |
| C5—H5B | 0.97 | C18—C19 | 1.382 (2) |
| C6—C7 | 1.403 (2) | C18—H18 | 0.93 |
| C6—H6 | 0.98 | C19—C20 | 1.399 (3) |
| C7—C8 | 1.402 (2) | C19—H19 | 0.93 |
| C7—C13 | 1.406 (2) | C20—C21 | 1.382 (2) |
| C8—F1B | 1.3282 | C20—H20 | 0.93 |
| C8—C10 | 1.389 (2) | C21—C22 | 1.405 (2) |
| C8—H8 | 0.93 | C21—H21 | 0.93 |
| C10—C11 | 1.402 (2) | C22—C23 | 1.476 (2) |
| C10—H10 | 0.93 | C23—O2 | 1.224 (2) |
| C11—C12 | 1.410 (2) | | |
| | | | |
| C6—C1—C2 | 112.53 (14) | C11—C10—H10 | 119.4 |
| C6—C1—H1A | 109.1 | C10—C11—C12 | 117.11 (14) |
| C2—C1—H1A | 109.1 | C10—C11—C14 | 125.82 (14) |
| C6—C1—H1B | 109.1 | C12—C11—C14 | 117.04 (14) |
| C2—C1—H1B | 109.1 | C13—C12—C11 | 120.46 (14) |
| H1A—C1—H1B | 107.8 | C13—C12—H12 | 119.8 |
| C1—C2—C3 | 112.13 (14) | C11—C12—H12 | 119.8 |
| C1—C2—H2A | 109.2 | F1A—C13—C12 | 118.33 (14) |
| C3—C2—H2A | 109.2 | F1A—C13—C7 | 118.06 (14) |
| C1—C2—H2B | 109.2 | C12—C13—C7 | 123.59 (14) |
| C3—C2—H2B | 109.2 | C12—C13—H13 | 118.2 |
| H2A—C2—H2B | 107.9 | C7—C13—H13 | 118.2 |
| C4—C3—C2 | 111.15 (15) | C15—C14—C11 | 131.10 (14) |
| C4—C3—H3A | 109.4 | C15—C14—H14 | 114.5 |
| C2—C3—H3A | 109.4 | C11—C14—H14 | 114.5 |
| C4—C3—H3B | 109.4 | C14—C15—C23 | 117.23 (14) |
| C2—C3—H3B | 109.4 | C14—C15—C16 | 125.62 (14) |
| H3A—C3—H3B | 108 | C23—C15—C16 | 117.08 (13) |
| C3—C4—C5 | 112.63 (15) | O1—C16—C15 | 114.82 (13) |
| C3—C4—H4A | 109.1 | O1—C16—H16A | 108.6 |
| C5—C4—H4A | 109.1 | C15—C16—H16A | 108.6 |

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| C3—C4—H4B | 109.1 | O1—C16—H16B | 108.6 |
| C5—C4—H4B | 109.1 | C15—C16—H16B | 108.6 |
| H4A—C4—H4B | 107.8 | H16A—C16—H16B | 107.5 |
| C6—C5—C4 | 111.53 (15) | O1—C17—C22 | 123.41 (14) |
| C6—C5—H5A | 109.3 | O1—C17—C18 | 116.25 (14) |
| C4—C5—H5A | 109.3 | C22—C17—C18 | 120.32 (15) |
| C6—C5—H5B | 109.3 | C19—C18—C17 | 119.57 (15) |
| C4—C5—H5B | 109.3 | C19—C18—H18 | 120.2 |
| H5A—C5—H5B | 108 | C17—C18—H18 | 120.2 |
| C7—C6—C5 | 117.07 (13) | C18—C19—C20 | 120.78 (16) |
| C7—C6—C1 | 116.12 (13) | C18—C19—H19 | 119.6 |
| C5—C6—C1 | 112.93 (13) | C20—C19—H19 | 119.6 |
| C7—C6—H6 | 102.6 | C21—C20—C19 | 119.60 (15) |
| C5—C6—H6 | 102.6 | C21—C20—H20 | 120.2 |
| C1—C6—H6 | 102.6 | C19—C20—H20 | 120.2 |
| C8—C7—C6 | 124.42 (14) | C20—C21—C22 | 120.61 (15) |
| C8—C7—C13 | 115.31 (14) | C20—C21—H21 | 119.7 |
| C6—C7—C13 | 120.25 (14) | C22—C21—H21 | 119.7 |
| F1B—C8—C10 | 114.28 (9) | C17—C22—C21 | 119.08 (14) |
| F1B—C8—C7 | 123.45 (9) | C17—C22—C23 | 120.42 (14) |
| C10—C8—C7 | 122.22 (14) | C21—C22—C23 | 120.41 (14) |
| C10—C8—H8 | 118.9 | O2—C23—C22 | 121.42 (15) |
| C7—C8—H8 | 118.9 | O2—C23—C15 | 122.84 (15) |
| C8—C10—C11 | 121.29 (14) | C22—C23—C15 | 115.73 (13) |
| C8—C10—H10 | 119.4 | C17—O1—C16 | 118.16 (12) |
| | | | |
| C6—C1—C2—C3 | 51.8 (2) | C10—C11—C14—C15 | 19.5 (3) |
| C1—C2—C3—C4 | −49.7 (2) | C12—C11—C14—C15 | −162.10 (17) |
| C2—C3—C4—C5 | 50.9 (2) | C11—C14—C15—C23 | −176.66 (15) |
| C3—C4—C5—C6 | −53.7 (2) | C11—C14—C15—C16 | 0.3 (3) |
| C4—C5—C6—C7 | −165.85 (15) | C14—C15—C16—O1 | 148.36 (16) |
| C4—C5—C6—C1 | 55.3 (2) | C23—C15—C16—O1 | −34.7 (2) |
| C2—C1—C6—C7 | 165.83 (15) | O1—C17—C18—C19 | 179.99 (15) |
| C2—C1—C6—C5 | −54.9 (2) | C22—C17—C18—C19 | 1.7 (3) |
| C5—C6—C7—C8 | −13.6 (2) | C17—C18—C19—C20 | 0.1 (3) |
| C1—C6—C7—C8 | 123.94 (17) | C18—C19—C20—C21 | −1.7 (3) |
| C5—C6—C7—C13 | 164.76 (15) | C19—C20—C21—C22 | 1.6 (2) |
| C1—C6—C7—C13 | −57.7 (2) | O1—C17—C22—C21 | −179.98 (14) |
| C6—C7—C8—F1B | −3.22 (19) | C18—C17—C22—C21 | −1.8 (2) |
| C13—C7—C8—F1B | 178.34 (9) | O1—C17—C22—C23 | −3.4 (2) |
| C6—C7—C8—C10 | 179.45 (15) | C18—C17—C22—C23 | 174.79 (15) |
| C13—C7—C8—C10 | 1.0 (2) | C20—C21—C22—C17 | 0.2 (2) |
| F1B—C8—C10—C11 | −177.69 (11) | C20—C21—C22—C23 | −176.43 (15) |
| C7—C8—C10—C11 | −0.1 (2) | C17—C22—C23—O2 | −175.13 (16) |
| C8—C10—C11—C12 | −0.3 (2) | C21—C22—C23—O2 | 1.4 (2) |
| C8—C10—C11—C14 | 178.12 (14) | C17—C22—C23—C15 | 4.4 (2) |
| C10—C11—C12—C13 | −0.2 (2) | C21—C22—C23—C15 | −179.02 (14) |
| C14—C11—C12—C13 | −178.77 (14) | C14—C15—C23—O2 | 11.4 (2) |
| C11—C12—C13—F1A | −177.15 (13) | C16—C15—C23—O2 | −165.74 (16) |

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| C11—C12—C13—C7 | 1.2 (2) | C14—C15—C23—C22 | −168.11 (14) |
| C8—C7—C13—F1A | 176.79 (13) | C16—C15—C23—C22 | 14.7 (2) |
| C6—C7—C13—F1A | −1.7 (2) | C22—C17—O1—C16 | −18.0 (2) |
| C8—C7—C13—C12 | −1.6 (2) | C18—C17—O1—C16 | 163.70 (15) |
| C6—C7—C13—C12 | 179.93 (14) | C15—C16—O1—C17 | 36.5 (2) |