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# (*E*)-9-(4-Fluorostyryl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-2*H*-xanthene-1,8-dione

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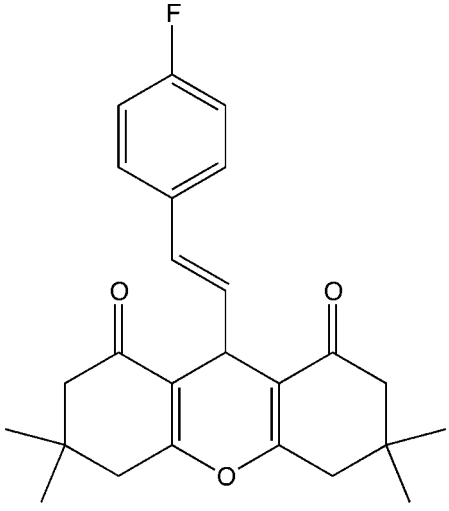
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.053; $wR$ factor = 0.169; data-to-parameter ratio = 17.8.

In the title compound, $C_{25}H_{27}FO_3$, each of the cyclohexenone rings adopts a half-chair conformation, whereas the six-membered pyran ring adopts a flattened boat conformation, with the O and methine C atoms deviating by 0.0769 (15) and 0.196 (2) Å, respectively, from the plane of the other four atoms (r.m.s. deviation = 0.004 Å). The C=C double bond adopts an *E* conformation. The dihedral angle between the benzene and pyran (all atoms) rings is 89.94 (10)°. In the crystal, weak C—H···O hydrogen bonds link the molecules into chains running parallel to the *b* axis.

## Related literature

For the crystal structures of xanthenes derivatives studied recently by our group, see: Cha *et al.* (2012, 2013); Lee *et al.* (2012).




## Experimental

### Crystal data

$C_{25}H_{27}FO_3$
$M_r$ = 394.48
Monoclinic, $P2_1/c$
$a$ = 5.9367 (7) Å
$b$ = 18.8521 (16) Å
$c$ = 19.3709 (16) Å
$\beta$ = 99.681 (3)°
$V$ = 2137.1 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
0.30 × 0.20 × 0.20 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Rigaku, 1995)
$T_{min}$ = 0.773, $T_{max}$ = 0.983
20480 measured reflections
4864 independent reflections
2857 reflections with $F^2 > 2\sigma(F^2)$
$R_{int}$ = 0.037

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.169
$S$ = 1.09
4864 reflections
274 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C22—H22$B$···O2$^{i}$ | 0.96 | 2.60 | 3.533 (4) | 163 |

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 2006); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *Il Milione* (Burla *et al.*, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2010); software used to prepare material for publication: *CrystalStructure*.

Financial support from the Korea Institute of Science and Technology (KIST) is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2106).

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# supporting information

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## (*E*)-9-(4-Fluorostyryl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-2*H*-xanthene-1,8-dione

**Jae Kyun Lee, Sun-Joon Min, Yong Seo Cho, Joo Hwan Cha and Sung Ok Won**

### S1. Comment

As part of our ongoing study of the substituent effect on the solid state structures of xanthene derivatives (Cha *et al.*, 2012; Lee *et al.*, 2012), we present here the crystal structure of the title compound (I) (Fig. 1).

The starting material, (*E*)-2.2-(3-(4-Fluorophenyl)prop-2-ene-1,1-diyl) bis(3-hydroxy-5,5-*δ*imethylcyclohex-2-enone) was prepared according to the reported method (Cha *et al.*, 2013). In (I) (Fig. 1), the bond lengths and angles are normal and correspond to those observed in related structures (Cha *et al.*, 2013). The dihedral angle between the benzene ring (C16 - C21) system and the pyran ring (C1—C2—C7—O3—C8—C13) is 89.94 (10)°. The C14=C15 double bond has an *E* conformation. All two cyclohexenone rings in (Fig. 1) display half-chair conformation, whereas the pyran ring adopts a boat conformation.

In the crystal, weak intermolecular C—H···O hydrogen bonds link molecules into chains running parallel to the *b* axis.

### S2. Experimental

To solution of (*E*)-2.2-(3-(4-Fluorophenyl)prop-2-ene-1,1-diyl)bis (3-hydroxy-5,5-dimethylcyclohex-2-enone) (1.25 mmol) was added methanol and catalytic amounts of sulfuric acid in under nitrogen atmosphere. After stirring for 4 h, the progress of reaction was monitored by TLC. The solvent was evaporated and the remaining residue dissolved in ethyl acetate. The mixture was neutralized with saturated sodium bicarbonate and the solution was extracted with ethyl acetate. The resulting residue solid was purified by recrystallization from ethanol and methylene chloride to afford yield 91%) colourless block type crystals suitable for X-ray analysis.

### S3. Refinement

All hydrogen atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.98 Å and *U*iso(H) = 1.2 or 1.5 *U*eq(C).

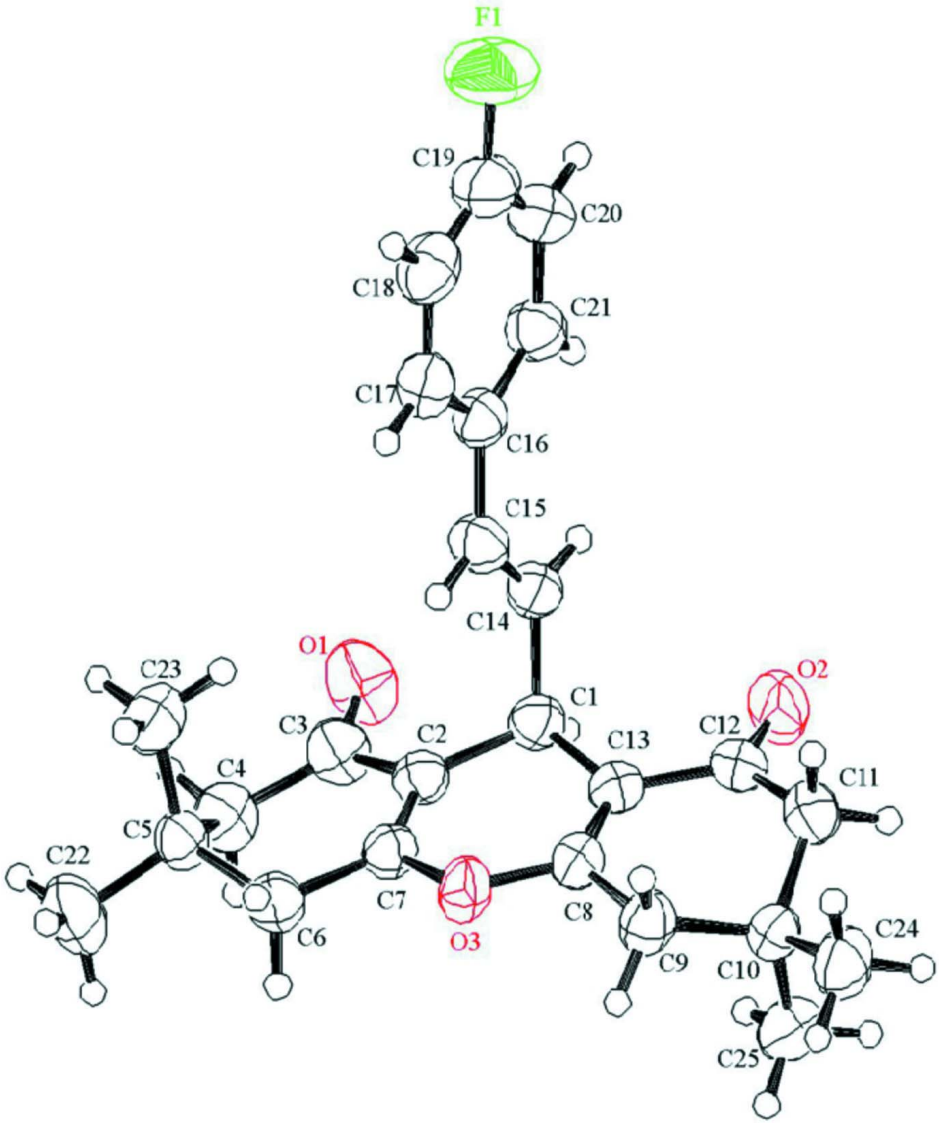


**Figure 1**

The molecular structure of (I) showing the atomic numbering and 50% probability displacement ellipsoid.

**(*E*)-9-(4-Fluorostyryl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-2*H*-xanthene-1,8-dione**

*Crystal data*

$C_{25}H_{27}FO_3$
$M_r = 394.48$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.9367\ (7)$ Å
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$c = 19.3709\ (16)$ Å
$\beta = 99.681\ (3)°$
$V = 2137.1\ (4)$ Å$^3$
$Z = 4$

$F(000) = 840.00$
$D_x = 1.226$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 12751 reflections
$\theta = 3.0–27.5°$
$\mu = 0.09$ mm$^{-1}$
$T = 296$ K
Chunk, colourless
0.30 × 0.20 × 0.20 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Rigaku, 1995)
$T_{min}$ = 0.773, $T_{max}$ = 0.983
20480 measured reflections
4864 independent reflections
2857 reflections with $F^2 > 2\sigma(F^2)$
$R_{int}$ = 0.037
$\theta_{max}$ = 27.5°
$h$ = −7→7
$k$ = −24→24
$l$ = −22→25

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.169
$S$ = 1.09
4864 reflections
274 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
$w = 1/[\sigma^2(F_o^2) + (0.0774P)^2 + 0.3562P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

*Special details*

**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 was performed using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on $F^2$. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F1 | 1.3085 (4) | 0.41875 (10) | 0.55088 (8) | 0.1071 (7) |
| O1 | 0.3415 (3) | 0.16938 (9) | 0.26856 (10) | 0.0755 (6) |
| O2 | 0.5001 (4) | 0.40605 (8) | 0.14354 (9) | 0.0743 (6) |
| O3 | 0.9010 (3) | 0.19315 (7) | 0.12327 (7) | 0.0508 (4) |
| C1 | 0.5863 (4) | 0.26673 (10) | 0.19791 (9) | 0.0457 (5) |
| C2 | 0.6201 (4) | 0.18746 (10) | 0.19814 (9) | 0.0427 (5) |
| C3 | 0.4790 (4) | 0.14307 (12) | 0.23554 (11) | 0.0541 (6) |
| C4 | 0.5029 (4) | 0.06354 (12) | 0.22949 (12) | 0.0591 (6) |
| C5 | 0.7461 (4) | 0.03924 (10) | 0.22594 (10) | 0.0451 (5) |
| C6 | 0.8316 (4) | 0.07994 (10) | 0.16669 (10) | 0.0484 (5) |
| C7 | 0.7745 (4) | 0.15633 (10) | 0.16515 (9) | 0.0424 (5) |
| C8 | 0.8474 (4) | 0.26351 (10) | 0.10936 (9) | 0.0449 (5) |
| C9 | 0.9782 (4) | 0.29226 (11) | 0.05617 (10) | 0.0517 (5) |
| C10 | 0.8696 (4) | 0.35891 (10) | 0.01931 (9) | 0.0469 (5) |
| C11 | 0.7974 (5) | 0.40786 (11) | 0.07479 (11) | 0.0592 (6) |
| C12 | 0.6512 (4) | 0.37327 (10) | 0.12129 (10) | 0.0512 (6) |
| C13 | 0.6981 (4) | 0.29901 (10) | 0.14075 (9) | 0.0445 (5) |

| | | | | |
|---|---|---|---|---|
| C14 | 0.6839 (4) | 0.30007 (11) | 0.26838 (10) | 0.0487 (5) |
| C15 | 0.8830 (4) | 0.28526 (11) | 0.30532 (11) | 0.0501 (5) |
| C16 | 0.9898 (4) | 0.31916 (10) | 0.37108 (10) | 0.0454 (5) |
| C17 | 1.2137 (4) | 0.30241 (11) | 0.40059 (11) | 0.0542 (6) |
| C18 | 1.3216 (5) | 0.33576 (13) | 0.46122 (12) | 0.0635 (6) |
| C19 | 1.2036 (5) | 0.38498 (13) | 0.49183 (12) | 0.0671 (7) |
| C20 | 0.9810 (5) | 0.40299 (12) | 0.46566 (12) | 0.0638 (7) |
| C21 | 0.8770 (4) | 0.36963 (11) | 0.40537 (11) | 0.0539 (6) |
| C22 | 0.7571 (6) | −0.03946 (12) | 0.21348 (15) | 0.0782 (8) |
| C23 | 0.8977 (5) | 0.05692 (13) | 0.29641 (11) | 0.0641 (7) |
| C24 | 1.0446 (5) | 0.39614 (12) | −0.01757 (12) | 0.0632 (7) |
| C25 | 0.6614 (5) | 0.33915 (13) | −0.03464 (11) | 0.0621 (6) |
| H1 | 0.4221 | 0.2767 | 0.1876 | 0.0549* |
| H4A | 0.4023 | 0.0474 | 0.1877 | 0.0710* |
| H4B | 0.4533 | 0.0413 | 0.2695 | 0.0710* |
| H6A | 0.9961 | 0.0747 | 0.1720 | 0.0581* |
| H6B | 0.7652 | 0.0589 | 0.1222 | 0.0581* |
| H9A | 0.9885 | 0.2560 | 0.0213 | 0.0620* |
| H9B | 1.1323 | 0.3034 | 0.0790 | 0.0620* |
| H11A | 0.9339 | 0.4264 | 0.1038 | 0.0711* |
| H11B | 0.7144 | 0.4478 | 0.0513 | 0.0711* |
| H17 | 1.2925 | 0.2683 | 0.3794 | 0.0651* |
| H18 | 1.4716 | 0.3246 | 0.4804 | 0.0762* |
| H20 | 0.9033 | 0.4365 | 0.4879 | 0.0766* |
| H21 | 0.7266 | 0.3812 | 0.3869 | 0.0646* |
| H22A | 0.6699 | −0.0508 | 0.1685 | 0.0938* |
| H22B | 0.6951 | −0.0643 | 0.2493 | 0.0938* |
| H22C | 0.9133 | −0.0534 | 0.2148 | 0.0938* |
| H23A | 0.8403 | 0.0328 | 0.3335 | 0.0769* |
| H23B | 0.8958 | 0.1072 | 0.3043 | 0.0769* |
| H23C | 1.0515 | 0.0418 | 0.2954 | 0.0769* |
| H24A | 0.9776 | 0.4381 | −0.0405 | 0.0758* |
| H24B | 1.0908 | 0.3647 | −0.0516 | 0.0758* |
| H24C | 1.1756 | 0.4090 | 0.0163 | 0.0758* |
| H25A | 0.5517 | 0.3152 | −0.0118 | 0.0745* |
| H25B | 0.7074 | 0.3084 | −0.0693 | 0.0745* |
| H25C | 0.5940 | 0.3814 | −0.0568 | 0.0745* |
| H14 | 0.606 (5) | 0.3358 (14) | 0.2853 (13) | 0.080 (8)* |
| H15 | 0.976 (5) | 0.2514 (13) | 0.2866 (13) | 0.070 (8)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.1157 (15) | 0.1169 (14) | 0.0759 (10) | −0.0103 (11) | −0.0212 (10) | −0.0327 (10) |
| O1 | 0.0723 (12) | 0.0670 (11) | 0.1011 (13) | 0.0029 (9) | 0.0546 (11) | −0.0011 (9) |
| O2 | 0.1033 (15) | 0.0543 (10) | 0.0726 (11) | 0.0236 (9) | 0.0359 (10) | 0.0042 (8) |
| O3 | 0.0574 (9) | 0.0486 (8) | 0.0522 (8) | 0.0101 (7) | 0.0257 (7) | 0.0112 (7) |
| C1 | 0.0488 (13) | 0.0489 (11) | 0.0410 (10) | 0.0065 (9) | 0.0121 (9) | −0.0005 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0447 (12) | 0.0447 (11) | 0.0398 (10) | 0.0003 (9) | 0.0109 (8) | −0.0013 (8) |
| C3 | 0.0488 (13) | 0.0572 (13) | 0.0605 (13) | −0.0001 (10) | 0.0210 (11) | −0.0010 (10) |
| C4 | 0.0537 (14) | 0.0595 (14) | 0.0660 (14) | −0.0074 (11) | 0.0149 (11) | 0.0005 (11) |
| C5 | 0.0478 (12) | 0.0414 (10) | 0.0488 (11) | −0.0023 (9) | 0.0157 (9) | 0.0013 (9) |
| C6 | 0.0528 (13) | 0.0471 (11) | 0.0486 (11) | 0.0026 (9) | 0.0183 (10) | 0.0003 (9) |
| C7 | 0.0451 (12) | 0.0461 (11) | 0.0380 (9) | 0.0001 (9) | 0.0128 (8) | 0.0019 (8) |
| C8 | 0.0515 (13) | 0.0440 (11) | 0.0394 (10) | 0.0016 (9) | 0.0084 (9) | 0.0041 (8) |
| C9 | 0.0548 (13) | 0.0534 (12) | 0.0495 (11) | 0.0022 (10) | 0.0162 (10) | 0.0080 (10) |
| C10 | 0.0560 (13) | 0.0445 (11) | 0.0399 (10) | −0.0030 (9) | 0.0073 (9) | 0.0033 (9) |
| C11 | 0.0814 (18) | 0.0426 (11) | 0.0550 (12) | −0.0065 (11) | 0.0153 (12) | −0.0009 (10) |
| C12 | 0.0691 (15) | 0.0439 (11) | 0.0413 (10) | 0.0030 (10) | 0.0112 (10) | −0.0063 (9) |
| C13 | 0.0527 (13) | 0.0450 (10) | 0.0364 (9) | 0.0026 (9) | 0.0100 (9) | −0.0000 (8) |
| C14 | 0.0591 (14) | 0.0477 (11) | 0.0412 (10) | 0.0116 (10) | 0.0143 (10) | −0.0020 (9) |
| C15 | 0.0520 (14) | 0.0481 (12) | 0.0519 (12) | 0.0063 (10) | 0.0133 (10) | −0.0070 (10) |
| C16 | 0.0503 (13) | 0.0432 (10) | 0.0444 (10) | 0.0008 (9) | 0.0124 (9) | 0.0033 (9) |
| C17 | 0.0538 (14) | 0.0541 (12) | 0.0558 (12) | 0.0031 (10) | 0.0121 (10) | 0.0050 (10) |
| C18 | 0.0553 (15) | 0.0706 (15) | 0.0611 (14) | −0.0025 (12) | 0.0000 (11) | 0.0090 (12) |
| C19 | 0.0787 (19) | 0.0662 (15) | 0.0524 (13) | −0.0144 (14) | −0.0006 (12) | −0.0048 (12) |
| C20 | 0.0752 (18) | 0.0623 (14) | 0.0541 (12) | 0.0026 (12) | 0.0113 (12) | −0.0123 (11) |
| C21 | 0.0537 (14) | 0.0561 (13) | 0.0521 (12) | 0.0046 (10) | 0.0098 (10) | −0.0038 (10) |
| C22 | 0.100 (3) | 0.0492 (13) | 0.0961 (19) | −0.0046 (13) | 0.0465 (17) | −0.0001 (13) |
| C23 | 0.0675 (17) | 0.0670 (15) | 0.0568 (13) | −0.0014 (12) | 0.0076 (12) | 0.0103 (12) |
| C24 | 0.0704 (17) | 0.0602 (14) | 0.0603 (13) | −0.0066 (12) | 0.0152 (12) | 0.0136 (11) |
| C25 | 0.0646 (16) | 0.0717 (15) | 0.0486 (12) | −0.0028 (12) | 0.0057 (11) | 0.0026 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F1—C19 | 1.365 (3) | C19—C20 | 1.376 (4) |
| O1—C3 | 1.224 (3) | C20—C21 | 1.378 (3) |
| O2—C12 | 1.226 (3) | C1—H1 | 0.980 |
| O3—C7 | 1.382 (3) | C4—H4A | 0.970 |
| O3—C8 | 1.380 (3) | C4—H4B | 0.970 |
| C1—C2 | 1.508 (3) | C6—H6A | 0.970 |
| C1—C13 | 1.511 (3) | C6—H6B | 0.970 |
| C1—C14 | 1.526 (3) | C9—H9A | 0.970 |
| C2—C3 | 1.460 (3) | C9—H9B | 0.970 |
| C2—C7 | 1.338 (3) | C11—H11A | 0.970 |
| C3—C4 | 1.512 (4) | C11—H11B | 0.970 |
| C4—C5 | 1.527 (4) | C14—H14 | 0.91 (3) |
| C5—C6 | 1.536 (3) | C15—H15 | 0.95 (3) |
| C5—C22 | 1.506 (3) | C17—H17 | 0.930 |
| C5—C23 | 1.540 (3) | C18—H18 | 0.930 |
| C6—C7 | 1.479 (3) | C20—H20 | 0.930 |
| C8—C9 | 1.492 (3) | C21—H21 | 0.930 |
| C8—C13 | 1.336 (3) | C22—H22A | 0.960 |
| C9—C10 | 1.533 (3) | C22—H22B | 0.960 |
| C10—C11 | 1.531 (3) | C22—H22C | 0.960 |
| C10—C24 | 1.527 (4) | C23—H23A | 0.960 |

| | | | |
|---|---|---|---|
| C10—C25 | 1.524 (3) | C23—H23B | 0.960 |
| C11—C12 | 1.501 (4) | C23—H23C | 0.960 |
| C12—C13 | 1.464 (3) | C24—H24A | 0.960 |
| C14—C15 | 1.305 (3) | C24—H24B | 0.960 |
| C15—C16 | 1.470 (3) | C24—H24C | 0.960 |
| C16—C17 | 1.392 (3) | C25—H25A | 0.960 |
| C16—C21 | 1.394 (3) | C25—H25B | 0.960 |
| C17—C18 | 1.390 (3) | C25—H25C | 0.960 |
| C18—C19 | 1.358 (4) | | |

| | | | |
|---|---|---|---|
| F1···C21 | 3.597 (3) | C1···H9B$^{ii}$ | 3.3111 |
| O1···C1 | 2.832 (3) | C3···H6A$^{ii}$ | 3.1946 |
| O1···C7 | 3.523 (3) | C3···H23C$^{ii}$ | 3.5247 |
| O1···C14 | 3.194 (3) | C4···H6A$^{ii}$ | 3.0348 |
| O2···C1 | 2.844 (3) | C4···H23C$^{ii}$ | 3.1830 |
| O2···C8 | 3.517 (3) | C6···H4A$^{iv}$ | 3.4001 |
| O2···C14 | 3.185 (3) | C6···H20$^{xi}$ | 3.5732 |
| O3···C1 | 2.900 (3) | C8···H1$^{iv}$ | 3.5015 |
| C2···C5 | 2.919 (3) | C8···H18$^{v}$ | 3.4780 |
| C2···C8 | 2.759 (3) | C9···H1$^{iv}$ | 3.3551 |
| C2···C15 | 3.009 (3) | C11···H23A$^{vi}$ | 3.4709 |
| C2···C23 | 3.367 (3) | C11···H23C$^{vi}$ | 3.5698 |
| C3···C6 | 2.918 (4) | C11···H24A$^{xii}$ | 3.3105 |
| C3···C14 | 3.222 (3) | C12···H9B$^{ii}$ | 3.3236 |
| C3···C23 | 3.036 (4) | C12···H24C$^{ii}$ | 3.2611 |
| C4···C7 | 2.809 (4) | C13···H9B$^{ii}$ | 3.3720 |
| C7···C13 | 2.755 (3) | C14···H17$^{ii}$ | 3.4730 |
| C7···C14 | 3.463 (3) | C14···H22B$^{iii}$ | 3.3846 |
| C7···C23 | 3.144 (3) | C15···H22C$^{vi}$ | 3.3203 |
| C8···C11 | 2.806 (3) | C15···H25B$^{ix}$ | 3.3106 |
| C8···C14 | 3.451 (3) | C16···H9A$^{ix}$ | 3.2382 |
| C8···C25 | 3.162 (3) | C16···H22A$^{vi}$ | 3.3468 |
| C9···C12 | 2.918 (4) | C16···H22C$^{vi}$ | 3.0316 |
| C10···C13 | 2.941 (3) | C16···H25B$^{ix}$ | 3.2531 |
| C12···C14 | 3.142 (3) | C17···H9A$^{ix}$ | 3.0860 |
| C12···C25 | 3.099 (3) | C17···H21$^{iv}$ | 3.4376 |
| C13···C15 | 3.203 (3) | C17···H22A$^{vi}$ | 3.1996 |
| C13···C25 | 3.452 (3) | C17···H22C$^{vi}$ | 3.5190 |
| C14···C21 | 3.009 (3) | C17···H24B$^{ix}$ | 3.3980 |
| C16···C19 | 2.761 (3) | C17···H25A$^{i}$ | 3.2675 |
| C17···C20 | 2.771 (4) | C17···H25B$^{i}$ | 3.5667 |
| C18···C21 | 2.754 (4) | C17···H14$^{iv}$ | 3.54 (3) |
| F1···C4$^{i}$ | 3.474 (3) | C18···H9A$^{ix}$ | 3.0056 |
| F1···C6$^{i}$ | 3.512 (3) | C18···H21$^{iv}$ | 3.1224 |
| F1···C7$^{i}$ | 3.535 (3) | C18···H22A$^{vi}$ | 3.3064 |
| O1···O3$^{ii}$ | 3.534 (3) | C18···H25A$^{i}$ | 3.1618 |
| O1···C23$^{ii}$ | 3.494 (4) | C19···H9A$^{ix}$ | 3.0437 |
| O2···C22$^{iii}$ | 3.533 (4) | C19···H20$^{x}$ | 3.4586 |

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|---|---|---|---|
| O3···O1$^{iv}$ | 3.534 (3) | C19···H22A$^{vi}$ | 3.5298 |
| C4···F1$^{v}$ | 3.474 (3) | C20···H6B$^{ix}$ | 3.5580 |
| C6···F1$^{v}$ | 3.512 (3) | C20···H9A$^{ix}$ | 3.1827 |
| C7···F1$^{v}$ | 3.535 (3) | C20···H18$^{ii}$ | 3.4206 |
| C16···C22$^{vi}$ | 3.588 (4) | C20···H20$^{x}$ | 3.1976 |
| C22···O2$^{vii}$ | 3.533 (4) | C21···H9A$^{ix}$ | 3.2544 |
| C22···C16$^{viii}$ | 3.588 (4) | C21···H18$^{ii}$ | 3.1313 |
| C23···O1$^{iv}$ | 3.494 (4) | C21···H22A$^{vi}$ | 3.5814 |
| F1···H18 | 2.5290 | C21···H22C$^{vi}$ | 3.1694 |
| F1···H20 | 2.5297 | C21···H25B$^{ix}$ | 3.5623 |
| O1···H1 | 2.6521 | C22···H21$^{vii}$ | 3.5200 |
| O1···H4A | 2.8387 | C22···H14$^{vii}$ | 3.19 (3) |
| O1···H4B | 2.5043 | C23···H4B$^{iv}$ | 3.4377 |
| O1···H23B | 3.4520 | C23···H11A$^{viii}$ | 3.1848 |
| O1···H14 | 3.50 (3) | C23···H24A$^{ix}$ | 3.1156 |
| O2···H1 | 2.6498 | C23···H24B$^{ix}$ | 3.3204 |
| O2···H11A | 2.8347 | C24···H11B$^{xii}$ | 3.3831 |
| O2···H11B | 2.4886 | C24···H23A$^{xi}$ | 3.2261 |
| O2···H25A | 3.5198 | C24···H23B$^{xi}$ | 3.4164 |
| O2···H14 | 3.02 (3) | C24···H24A$^{xii}$ | 3.3320 |
| O3···H6A | 2.4523 | C24···H25A$^{iv}$ | 3.3600 |
| O3···H6B | 2.6557 | C24···H25C$^{iv}$ | 3.4827 |
| O3···H9A | 2.4322 | C25···H17$^{v}$ | 3.2327 |
| O3···H9B | 2.7096 | C25···H18$^{v}$ | 3.3155 |
| O3···H15 | 3.31 (3) | C25···H24B$^{ii}$ | 3.3827 |
| C1···H15 | 2.65 (3) | C25···H24C$^{ii}$ | 3.4616 |
| C2···H4A | 2.9317 | H1···O3$^{ii}$ | 3.5083 |
| C2···H4B | 3.3091 | H1···C8$^{ii}$ | 3.5015 |
| C2···H6A | 3.1832 | H1···C9$^{ii}$ | 3.3551 |
| C2···H6B | 3.0345 | H1···H9B$^{ii}$ | 2.5347 |
| C2···H23B | 2.8394 | H1···H22B$^{iii}$ | 3.3533 |
| C2···H14 | 3.27 (3) | H1···H15$^{ii}$ | 3.5543 |
| C2···H15 | 2.76 (3) | H4A···F1$^{v}$ | 2.6922 |
| C3···H1 | 2.6867 | H4A···C6$^{ii}$ | 3.4001 |
| C3···H6B | 3.3883 | H4A···H6A$^{ii}$ | 2.4346 |
| C3···H23A | 3.3393 | H4A···H21$^{vii}$ | 3.4827 |
| C3···H23B | 2.6914 | H4A···H22C$^{ii}$ | 3.5817 |
| C3···H15 | 3.59 (3) | H4A···H23C$^{ii}$ | 3.1875 |
| C4···H6A | 3.3095 | H4B···O2$^{vii}$ | 3.0419 |
| C4···H6B | 2.7999 | H4B···C23$^{ii}$ | 3.4377 |
| C4···H22A | 2.7237 | H4B···H6A$^{ii}$ | 3.0997 |
| C4···H22B | 2.6671 | H4B···H23C$^{ii}$ | 2.5189 |
| C4···H22C | 3.3330 | H6A···F1$^{xi}$ | 3.2287 |
| C4···H23A | 2.6551 | H6A···O1$^{iv}$ | 3.0975 |
| C4···H23B | 2.6606 | H6A···C3$^{iv}$ | 3.1946 |
| C4···H23C | 3.3172 | H6A···C4$^{iv}$ | 3.0348 |
| C6···H4A | 2.7173 | H6A···H4A$^{iv}$ | 2.4346 |
| C6···H4B | 3.3234 | H6A···H4B$^{iv}$ | 3.0997 |

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|---|---|---|---|
| C6···H22A | 2.6471 | H6A···H20$^{xi}$ | 3.5224 |
| C6···H22B | 3.3240 | H6B···F1$^{v}$ | 2.8599 |
| C6···H22C | 2.6962 | H6B···C20$^{xi}$ | 3.5580 |
| C6···H23A | 3.3434 | H6B···H20$^{xi}$ | 2.8574 |
| C6···H23B | 2.6773 | H9A···C16$^{xi}$ | 3.2382 |
| C6···H23C | 2.7096 | H9A···C17$^{xi}$ | 3.0860 |
| C7···H1 | 3.1660 | H9A···C18$^{xi}$ | 3.0056 |
| C7···H4A | 3.1005 | H9A···C19$^{xi}$ | 3.0437 |
| C7···H23B | 2.8257 | H9A···C20$^{xi}$ | 3.1827 |
| C7···H23C | 3.5123 | H9A···C21$^{xi}$ | 3.2544 |
| C7···H15 | 3.04 (3) | H9A···H17$^{xi}$ | 3.5637 |
| C8···H1 | 3.1658 | H9A···H18$^{v}$ | 3.3955 |
| C8···H11A | 3.1173 | H9A···H18$^{xi}$ | 3.4535 |
| C8···H25A | 2.8550 | H9B···O2$^{iv}$ | 3.0258 |
| C8···H25B | 3.5231 | H9B···C1$^{iv}$ | 3.3111 |
| C8···H15 | 3.40 (3) | H9B···C12$^{iv}$ | 3.3236 |
| C9···H11A | 2.7191 | H9B···C13$^{iv}$ | 3.3720 |
| C9···H11B | 3.3179 | H9B···H1$^{iv}$ | 2.5347 |
| C9···H24A | 3.3260 | H9B···H25A$^{iv}$ | 3.2878 |
| C9···H24B | 2.6728 | H11A···O2$^{iv}$ | 3.3418 |
| C9···H24C | 2.6682 | H11A···C23$^{vi}$ | 3.1848 |
| C9···H25A | 2.6849 | H11A···H22B$^{vi}$ | 3.2970 |
| C9···H25B | 2.6957 | H11A···H22C$^{vi}$ | 3.4992 |
| C9···H25C | 3.3375 | H11A···H23A$^{vi}$ | 2.5987 |
| C11···H9A | 3.3094 | H11A···H23C$^{vi}$ | 2.9148 |
| C11···H9B | 2.7892 | H11A···H24A$^{xii}$ | 2.9207 |
| C11···H24A | 2.6947 | H11B···C24$^{xii}$ | 3.3831 |
| C11···H24B | 3.3354 | H11B···H11B$^{xiii}$ | 3.5508 |
| C11···H24C | 2.6797 | H11B···H23A$^{vi}$ | 3.5428 |
| C11···H25A | 2.6776 | H11B···H23C$^{vi}$ | 3.5355 |
| C11···H25B | 3.3292 | H11B···H24A$^{xii}$ | 2.8542 |
| C11···H25C | 2.6784 | H11B···H24C$^{ii}$ | 3.2402 |
| C12···H1 | 2.7208 | H11B···H24C$^{xii}$ | 3.1172 |
| C12···H9B | 3.3688 | H17···O1$^{iv}$ | 2.8952 |
| C12···H25A | 2.7712 | H17···C14$^{iv}$ | 3.4730 |
| C12···H25C | 3.4135 | H17···C25$^{i}$ | 3.2327 |
| C12···H14 | 3.31 (3) | H17···H9A$^{ix}$ | 3.5637 |
| C13···H9A | 3.2125 | H17···H21$^{iv}$ | 3.3260 |
| C13···H9B | 3.0200 | H17···H22A$^{vi}$ | 3.5506 |
| C13···H11A | 2.9274 | H17···H24B$^{ix}$ | 3.1705 |
| C13···H11B | 3.3065 | H17···H25A$^{i}$ | 2.8640 |
| C13···H25A | 2.9519 | H17···H25B$^{i}$ | 2.8858 |
| C13···H14 | 3.02 (3) | H17···H25C$^{i}$ | 3.4576 |
| C13···H15 | 3.15 (3) | H17···H14$^{iv}$ | 3.0895 |
| C14···H21 | 2.7346 | H18···O3$^{i}$ | 3.4484 |
| C15···H1 | 3.2578 | H18···C8$^{i}$ | 3.4780 |
| C15···H17 | 2.6261 | H18···C20$^{iv}$ | 3.4206 |
| C15···H21 | 2.6687 | H18···C21$^{iv}$ | 3.1313 |

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|---|---|---|---|
| C15···H23B | 3.3580 | H18···C25$^{i}$ | 3.3155 |
| C16···H18 | 3.2625 | H18···H9A$^{ix}$ | 3.4535 |
| C16···H20 | 3.2668 | H18···H9A$^{i}$ | 3.3955 |
| C16···H14 | 2.60 (3) | H18···H20$^{iv}$ | 3.3044 |
| C17···H21 | 3.2216 | H18···H21$^{iv}$ | 2.7628 |
| C17···H15 | 2.60 (3) | H18···H25A$^{i}$ | 2.6772 |
| C18···H20 | 3.2365 | H18···H25B$^{i}$ | 3.1027 |
| C19···H17 | 3.2011 | H20···F1$^{x}$ | 3.0448 |
| C19···H21 | 3.1964 | H20···O3$^{ix}$ | 3.5868 |
| C20···H18 | 3.2361 | H20···C6$^{ix}$ | 3.5732 |
| C21···H17 | 3.2251 | H20···C19$^{x}$ | 3.4586 |
| C21···H14 | 2.67 (3) | H20···C20$^{x}$ | 3.1976 |
| C21···H15 | 3.33 (3) | H20···H6A$^{ix}$ | 3.5224 |
| C22···H4A | 2.6483 | H20···H6B$^{ix}$ | 2.8574 |
| C22···H4B | 2.7210 | H20···H18$^{ii}$ | 3.3044 |
| C22···H6A | 2.7709 | H20···H20$^{x}$ | 2.6610 |
| C22···H6B | 2.5677 | H21···C17$^{ii}$ | 3.4376 |
| C22···H23A | 2.6688 | H21···C18$^{ii}$ | 3.1224 |
| C22···H23B | 3.3055 | H21···C22$^{iii}$ | 3.5200 |
| C22···H23C | 2.6427 | H21···H4A$^{iii}$ | 3.4827 |
| C23···H4A | 3.3211 | H21···H17$^{ii}$ | 3.3260 |
| C23···H4B | 2.6184 | H21···H18$^{ii}$ | 2.7628 |
| C23···H6A | 2.5950 | H21···H22A$^{iii}$ | 2.7368 |
| C23···H6B | 3.3338 | H21···H22B$^{iii}$ | 3.4731 |
| C23···H22A | 3.3113 | H21···H22C$^{vi}$ | 3.3746 |
| C23···H22B | 2.6714 | H22A···C16$^{viii}$ | 3.3468 |
| C23···H22C | 2.6239 | H22A···C17$^{viii}$ | 3.1996 |
| C24···H9A | 2.7833 | H22A···C18$^{viii}$ | 3.3064 |
| C24···H9B | 2.5485 | H22A···C19$^{viii}$ | 3.5298 |
| C24···H11A | 2.6092 | H22A···C21$^{viii}$ | 3.5814 |
| C24···H11B | 2.7298 | H22A···H17$^{viii}$ | 3.5506 |
| C24···H25A | 3.3190 | H22A···H21$^{vii}$ | 2.7368 |
| C24···H25B | 2.6590 | H22A···H14$^{vii}$ | 2.9242 |
| C24···H25C | 2.6697 | H22B···O2$^{vii}$ | 2.6029 |
| C25···H9A | 2.5878 | H22B···C14$^{vii}$ | 3.3846 |
| C25···H9B | 3.3230 | H22B···H1$^{vii}$ | 3.3533 |
| C25···H11A | 3.3249 | H22B···H11A$^{viii}$ | 3.2970 |
| C25···H11B | 2.6250 | H22B···H21$^{vii}$ | 3.4731 |
| C25···H24A | 2.6618 | H22B···H14$^{vii}$ | 2.6050 |
| C25···H24B | 2.6684 | H22C···C15$^{viii}$ | 3.3203 |
| C25···H24C | 3.3184 | H22C···C16$^{viii}$ | 3.0316 |
| H1···H14 | 2.3060 | H22C···C17$^{viii}$ | 3.5190 |
| H1···H15 | 3.5473 | H22C···C21$^{viii}$ | 3.1694 |
| H4A···H6B | 2.6867 | H22C···H4A$^{iv}$ | 3.5817 |
| H4A···H22A | 2.5078 | H22C···H11A$^{viii}$ | 3.4992 |
| H4A···H22B | 2.8608 | H22C···H21$^{viii}$ | 3.3746 |
| H4A···H22C | 3.5429 | H22C···H14$^{viii}$ | 3.5369 |
| H4A···H23A | 3.5130 | H23A···O2$^{vii}$ | 3.2088 |

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|---|---|---|---|
| H4A···H23B | 3.5669 | H23A···C11$^{viii}$ | 3.4709 |
| H4B···H22A | 3.0561 | H23A···C24$^{ix}$ | 3.2261 |
| H4B···H22B | 2.5231 | H23A···H11A$^{viii}$ | 2.5987 |
| H4B···H22C | 3.5691 | H23A···H11B$^{viii}$ | 3.5428 |
| H4B···H23A | 2.4253 | H23A···H24A$^{ix}$ | 2.4997 |
| H4B···H23B | 2.8818 | H23A···H24B$^{ix}$ | 3.1267 |
| H4B···H23C | 3.5018 | H23A···H25C$^{ix}$ | 3.2102 |
| H6A···H22A | 3.0515 | H23B···O1$^{iv}$ | 3.0772 |
| H6A···H22C | 2.6270 | H23B···C24$^{ix}$ | 3.4164 |
| H6A···H23A | 3.4987 | H23B···H24A$^{ix}$ | 3.0844 |
| H6A···H23B | 2.7933 | H23B···H24B$^{ix}$ | 2.8856 |
| H6A···H23C | 2.4373 | H23B···H25B$^{ix}$ | 3.2722 |
| H6B···H22A | 2.3597 | H23B···H25C$^{ix}$ | 3.4810 |
| H6B···H22B | 3.4599 | H23C···O1$^{iv}$ | 3.0534 |
| H6B···H22C | 2.8171 | H23C···C3$^{iv}$ | 3.5247 |
| H6B···H23B | 3.5981 | H23C···C4$^{iv}$ | 3.1830 |
| H6B···H23C | 3.5109 | H23C···C11$^{viii}$ | 3.5698 |
| H9A···H24B | 2.6192 | H23C···H4A$^{iv}$ | 3.1875 |
| H9A···H24C | 3.0991 | H23C···H4B$^{iv}$ | 2.5189 |
| H9A···H25A | 2.7968 | H23C···H11A$^{viii}$ | 2.9148 |
| H9A···H25B | 2.4202 | H23C···H11B$^{viii}$ | 3.5355 |
| H9A···H25C | 3.4894 | H23C···H24A$^{ix}$ | 3.3030 |
| H9B···H11A | 2.6795 | H23C···H24B$^{ix}$ | 3.4221 |
| H9B···H24A | 3.4538 | H24A···C11$^{xii}$ | 3.3105 |
| H9B···H24B | 2.7544 | H24A···C23$^{xi}$ | 3.1156 |
| H9B···H24C | 2.3679 | H24A···C24$^{xii}$ | 3.3320 |
| H9B···H25B | 3.4901 | H24A···H11A$^{xii}$ | 2.9207 |
| H11A···H24A | 2.8602 | H24A···H11B$^{xii}$ | 2.8542 |
| H11A···H24B | 3.4971 | H24A···H23A$^{xi}$ | 2.4997 |
| H11A···H24C | 2.4211 | H24A···H23B$^{xi}$ | 3.0844 |
| H11A···H25A | 3.5841 | H24A···H23C$^{xi}$ | 3.3030 |
| H11A···H25C | 3.5165 | H24A···H24A$^{xii}$ | 2.8015 |
| H11B···H24A | 2.5642 | H24A···H24C$^{xii}$ | 3.0825 |
| H11B···H24B | 3.5944 | H24B···C17$^{xi}$ | 3.3980 |
| H11B···H24C | 3.0192 | H24B···C23$^{xi}$ | 3.3204 |
| H11B···H25A | 2.8774 | H24B···C25$^{iv}$ | 3.3827 |
| H11B···H25B | 3.5111 | H24B···H17$^{xi}$ | 3.1705 |
| H11B···H25C | 2.4423 | H24B···H23A$^{xi}$ | 3.1267 |
| H17···H18 | 2.3213 | H24B···H23B$^{xi}$ | 2.8856 |
| H17···H15 | 2.3945 | H24B···H23C$^{xi}$ | 3.4221 |
| H20···H21 | 2.3081 | H24B···H25A$^{iv}$ | 2.8715 |
| H21···H14 | 2.1556 | H24B···H25C$^{iv}$ | 3.0227 |
| H21···H15 | 3.5935 | H24C···O2$^{iv}$ | 2.8628 |
| H22A···H23A | 3.5554 | H24C···C12$^{iv}$ | 3.2611 |
| H22A···H23C | 3.5135 | H24C···C25$^{iv}$ | 3.4616 |
| H22B···H23A | 2.5079 | H24C···H11B$^{iv}$ | 3.2402 |
| H22B···H23B | 3.5474 | H24C···H11B$^{xii}$ | 3.1172 |
| H22B···H23C | 2.9393 | H24C···H24A$^{xii}$ | 3.0825 |

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|---|---|---|---|
| H22C···H23A | 2.9083 | H24C···H25A$^{iv}$ | 2.9694 |
| H22C···H23B | 3.4988 | H24C···H25C$^{iv}$ | 3.1036 |
| H22C···H23C | 2.4290 | H25A···C17$^{v}$ | 3.2675 |
| H23B···H15 | 2.7912 | H25A···C18$^{v}$ | 3.1618 |
| H24A···H25A | 3.5416 | H25A···C24$^{ii}$ | 3.3600 |
| H24A···H25B | 2.9248 | H25A···H9B$^{ii}$ | 3.2878 |
| H24A···H25C | 2.4867 | H25A···H17$^{v}$ | 2.8640 |
| H24B···H25A | 3.5415 | H25A···H18$^{v}$ | 2.6772 |
| H24B···H25B | 2.4823 | H25A···H24B$^{ii}$ | 2.8715 |
| H24B···H25C | 2.9505 | H25A···H24C$^{ii}$ | 2.9694 |
| H24C···H25B | 3.5378 | H25B···O1$^{xi}$ | 3.5309 |
| H24C···H25C | 3.5428 | H25B···C15$^{xi}$ | 3.3106 |
| H14···H15 | 2.71 (4) | H25B···C16$^{xi}$ | 3.2531 |
| F1···H4A$^{i}$ | 2.6922 | H25B···C17$^{v}$ | 3.5667 |
| F1···H6A$^{ix}$ | 3.2287 | H25B···C21$^{xi}$ | 3.5623 |
| F1···H6B$^{i}$ | 2.8599 | H25B···H17$^{v}$ | 2.8858 |
| F1···H20$^{x}$ | 3.0448 | H25B···H18$^{v}$ | 3.1027 |
| O1···H6A$^{ii}$ | 3.0975 | H25B···H23B$^{xi}$ | 3.2722 |
| O1···H17$^{ii}$ | 2.8952 | H25C···O1$^{xi}$ | 3.5911 |
| O1···H23B$^{ii}$ | 3.0772 | H25C···C24$^{ii}$ | 3.4827 |
| O1···H23C$^{ii}$ | 3.0534 | H25C···H17$^{v}$ | 3.4576 |
| O1···H25B$^{ix}$ | 3.5309 | H25C···H23A$^{xi}$ | 3.2102 |
| O1···H25C$^{ix}$ | 3.5911 | H25C···H23B$^{xi}$ | 3.4810 |
| O1···H15$^{ii}$ | 2.74 (3) | H25C···H24B$^{ii}$ | 3.0227 |
| O2···H4B$^{iii}$ | 3.0419 | H25C···H24C$^{ii}$ | 3.1036 |
| O2···H9B$^{ii}$ | 3.0258 | H14···C17$^{ii}$ | 3.54 (3) |
| O2···H11A$^{ii}$ | 3.3418 | H14···C22$^{iii}$ | 3.19 (3) |
| O2···H22B$^{iii}$ | 2.6029 | H14···H17$^{ii}$ | 3.0895 |
| O2···H23A$^{iii}$ | 3.2088 | H14···H22A$^{iii}$ | 2.9242 |
| O2···H24C$^{ii}$ | 2.8628 | H14···H22B$^{iii}$ | 2.6050 |
| O3···H1$^{iv}$ | 3.5083 | H14···H22C$^{vi}$ | 3.5369 |
| O3···H18$^{v}$ | 3.4484 | H15···O1$^{iv}$ | 2.74 (3) |
| O3···H20$^{xi}$ | 3.5868 | H15···H1$^{iv}$ | 3.5543 |

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|---|---|---|---|
| C7—O3—C8 | 117.86 (16) | C5—C4—H4A | 108.816 |
| C2—C1—C13 | 109.06 (17) | C5—C4—H4B | 108.809 |
| C2—C1—C14 | 112.04 (15) | H4A—C4—H4B | 107.675 |
| C13—C1—C14 | 110.00 (17) | C5—C6—H6A | 108.873 |
| C1—C2—C3 | 118.84 (18) | C5—C6—H6B | 108.870 |
| C1—C2—C7 | 122.35 (18) | C7—C6—H6A | 108.879 |
| C3—C2—C7 | 118.81 (18) | C7—C6—H6B | 108.878 |
| O1—C3—C2 | 121.1 (2) | H6A—C6—H6B | 107.714 |
| O1—C3—C4 | 121.5 (3) | C8—C9—H9A | 108.964 |
| C2—C3—C4 | 117.4 (2) | C8—C9—H9B | 108.967 |
| C3—C4—C5 | 113.74 (19) | C10—C9—H9A | 108.960 |
| C4—C5—C6 | 108.50 (17) | C10—C9—H9B | 108.949 |
| C4—C5—C22 | 111.7 (2) | H9A—C9—H9B | 107.764 |
| C4—C5—C23 | 108.13 (18) | C10—C11—H11A | 108.599 |

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| C6—C5—C22 | 110.10 (19) | C10—C11—H11B | 108.596 |
| C6—C5—C23 | 109.69 (17) | C12—C11—H11A | 108.585 |
| C22—C5—C23 | 108.70 (18) | C12—C11—H11B | 108.593 |
| C5—C6—C7 | 113.47 (18) | H11A—C11—H11B | 107.567 |
| O3—C7—C2 | 122.94 (18) | C1—C14—H14 | 119.2 (16) |
| O3—C7—C6 | 110.85 (17) | C15—C14—H14 | 115.5 (16) |
| C2—C7—C6 | 126.20 (19) | C14—C15—H15 | 117.5 (14) |
| O3—C8—C9 | 110.75 (17) | C16—C15—H15 | 115.4 (14) |
| O3—C8—C13 | 122.79 (18) | C16—C17—H17 | 119.438 |
| C9—C8—C13 | 126.46 (18) | C18—C17—H17 | 119.442 |
| C8—C9—C10 | 113.10 (19) | C17—C18—H18 | 120.662 |
| C9—C10—C11 | 108.21 (16) | C19—C18—H18 | 120.663 |
| C9—C10—C24 | 109.18 (19) | C19—C20—H20 | 121.137 |
| C9—C10—C25 | 110.37 (17) | C21—C20—H20 | 121.142 |
| C11—C10—C24 | 110.12 (18) | C16—C21—H21 | 118.893 |
| C11—C10—C25 | 109.78 (19) | C20—C21—H21 | 118.900 |
| C24—C10—C25 | 109.18 (17) | C5—C22—H22A | 109.474 |
| C10—C11—C12 | 114.68 (17) | C5—C22—H22B | 109.466 |
| O2—C12—C11 | 121.55 (19) | C5—C22—H22C | 109.466 |
| O2—C12—C13 | 120.7 (2) | H22A—C22—H22B | 109.474 |
| C11—C12—C13 | 117.8 (2) | H22A—C22—H22C | 109.478 |
| C1—C13—C8 | 122.58 (18) | H22B—C22—H22C | 109.470 |
| C1—C13—C12 | 119.06 (18) | C5—C23—H23A | 109.470 |
| C8—C13—C12 | 118.28 (19) | C5—C23—H23B | 109.469 |
| C1—C14—C15 | 125.1 (2) | C5—C23—H23C | 109.469 |
| C14—C15—C16 | 126.9 (2) | H23A—C23—H23B | 109.474 |
| C15—C16—C17 | 120.00 (19) | H23A—C23—H23C | 109.481 |
| C15—C16—C21 | 122.54 (19) | H23B—C23—H23C | 109.464 |
| C17—C16—C21 | 117.45 (18) | C10—C24—H24A | 109.469 |
| C16—C17—C18 | 121.1 (2) | C10—C24—H24B | 109.475 |
| C17—C18—C19 | 118.7 (3) | C10—C24—H24C | 109.473 |
| F1—C19—C18 | 119.2 (3) | H24A—C24—H24B | 109.474 |
| F1—C19—C20 | 117.9 (3) | H24A—C24—H24C | 109.474 |
| C18—C19—C20 | 122.8 (3) | H24B—C24—H24C | 109.463 |
| C19—C20—C21 | 117.7 (3) | C10—C25—H25A | 109.471 |
| C16—C21—C20 | 122.2 (2) | C10—C25—H25B | 109.473 |
| C2—C1—H1 | 108.563 | C10—C25—H25C | 109.459 |
| C13—C1—H1 | 108.543 | H25A—C25—H25B | 109.473 |
| C14—C1—H1 | 108.553 | H25A—C25—H25C | 109.466 |
| C3—C4—H4A | 108.819 | H25B—C25—H25C | 109.484 |
| C3—C4—H4B | 108.810 | | |

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| C7—O3—C8—C9 | −172.44 (13) | O3—C8—C9—C10 | 159.36 (13) |
| C7—O3—C8—C13 | 7.8 (3) | O3—C8—C13—C1 | 4.2 (3) |
| C8—O3—C7—C2 | −7.0 (3) | O3—C8—C13—C12 | −179.08 (14) |
| C8—O3—C7—C6 | 172.08 (13) | C9—C8—C13—C1 | −175.50 (15) |
| C2—C1—C13—C8 | −15.0 (3) | C9—C8—C13—C12 | 1.2 (3) |
| C2—C1—C13—C12 | 168.36 (14) | C13—C8—C9—C10 | −20.9 (3) |

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| C13—C1—C2—C3 | −164.10 (14) | C8—C9—C10—C11 | 44.1 (2) |
| C13—C1—C2—C7 | 15.7 (3) | C8—C9—C10—C24 | 163.94 (14) |
| C2—C1—C14—C15 | 44.9 (3) | C8—C9—C10—C25 | −76.05 (19) |
| C14—C1—C2—C3 | 73.9 (2) | C9—C10—C11—C12 | −52.5 (3) |
| C14—C1—C2—C7 | −106.30 (19) | C24—C10—C11—C12 | −171.74 (16) |
| C13—C1—C14—C15 | −76.6 (3) | C25—C10—C11—C12 | 68.0 (2) |
| C14—C1—C13—C8 | 108.27 (19) | C10—C11—C12—O2 | −145.70 (18) |
| C14—C1—C13—C12 | −68.4 (2) | C10—C11—C12—C13 | 35.6 (3) |
| C1—C2—C3—O1 | −2.8 (3) | O2—C12—C13—C1 | −10.2 (3) |
| C1—C2—C3—C4 | 174.82 (14) | O2—C12—C13—C8 | 172.99 (17) |
| C1—C2—C7—O3 | −5.9 (3) | C11—C12—C13—C1 | 168.47 (15) |
| C1—C2—C7—C6 | 175.25 (14) | C11—C12—C13—C8 | −8.3 (3) |
| C3—C2—C7—O3 | 173.98 (15) | C1—C14—C15—C16 | 175.85 (18) |
| C3—C2—C7—C6 | −4.9 (3) | C14—C15—C16—C17 | −173.4 (2) |
| C7—C2—C3—O1 | 177.32 (16) | C14—C15—C16—C21 | 5.1 (4) |
| C7—C2—C3—C4 | −5.0 (3) | C15—C16—C17—C18 | 177.44 (18) |
| O1—C3—C4—C5 | −146.87 (19) | C15—C16—C21—C20 | −177.67 (18) |
| C2—C3—C4—C5 | 35.5 (3) | C17—C16—C21—C20 | 0.9 (3) |
| C3—C4—C5—C6 | −53.4 (2) | C21—C16—C17—C18 | −1.1 (3) |
| C3—C4—C5—C22 | −174.90 (15) | C16—C17—C18—C19 | 0.5 (4) |
| C3—C4—C5—C23 | 65.5 (2) | C17—C18—C19—F1 | −179.2 (2) |
| C4—C5—C6—C7 | 43.3 (2) | C17—C18—C19—C20 | 0.4 (4) |
| C22—C5—C6—C7 | 165.83 (17) | F1—C19—C20—C21 | 178.92 (19) |
| C23—C5—C6—C7 | −74.6 (2) | C18—C19—C20—C21 | −0.7 (4) |
| C5—C6—C7—O3 | 165.12 (14) | C19—C20—C21—C16 | 0.0 (4) |
| C5—C6—C7—C2 | −15.9 (3) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C22—H22*B*···O2$^{vii}$ | 0.96 | 2.60 | 3.533 (4) | 163 |

Symmetry code: (vii) −*x*+1, *y*−1/2, −*z*+1/2.