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

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

In the title compound, C₂₅H₂₇FO₃, each of the cyclohexenone rings adopts a half-chair conformation, whereas the sixmembered 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).

20480 measured reflections

 $R_{\rm int} = 0.037$

4864 independent reflections 2857 reflections with $F^2 > 2\sigma(F^2)$

Experimental

Crystal data

C25H27FO3	V = 2137.1 (4) Å ³
$M_r = 394.48$	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 5.9367 (7) Å	$\mu = 0.09 \text{ mm}^{-1}$
b = 18.8521 (16) Å	T = 296 K
c = 19.3709 (16) Å	$0.30 \times 0.20 \times 0.20$ mm
$\beta = 99.681 \ (3)^{\circ}$	

Data collection

Rigaku R-AXIS RAPID diffractometer Absorption correction: multi-scan (ABSCOR; Rigaku, 1995) $T_{\min} = 0.773, \ \tilde{T}_{\max} = 0.983$

Refinement

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

Table 1

Hydrogen-bond geometry (Å, °).

 $D - H \cdot \cdot \cdot A$ $D - H \cdot \cdot \cdot A$ D - H $H \cdot \cdot \cdot A$ $D \cdots A$ $C22 - H22B \cdot \cdot \cdot O2^{i}$ 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.

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

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supporting information

Acta Cryst. (2013). E69, o985 [doi:10.1107/S1600536813014049]

(*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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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 Uiso(H) = 1.2 or 1.5 Ueq(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-2H-xanthene-1,8-dione

Crystal data	
C ₂₅ H ₂₇ FO ₃	F(000) = 840.00
$M_r = 394.48$	$D_{\rm x} = 1.226 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Hall symbol: -P 2ybc	Cell parameters from 12751 reflections
a = 5.9367 (7) Å	$\theta = 3.0-27.5^{\circ}$
b = 18.8521 (16) Å	$\mu = 0.09 \text{ mm}^{-1}$
c = 19.3709 (16) Å	T = 296 K
$\beta = 99.681 \ (3)^{\circ}$	Chunk, colourless
V = 2137.1 (4) Å ³	$0.30 \times 0.20 \times 0.20$ mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer Detector resolution: 10.000 pixels mm ⁻¹ ω scans Absorption correction: multi-scan (<i>ABSCOR</i> ; Rigaku, 1995) $T_{\rm min} = 0.773, T_{\rm max} = 0.983$ 20480 measured reflections	4864 independent reflections 2857 reflections with $F^2 > 2\sigma(F^2)$ $R_{int} = 0.037$ $\theta_{max} = 27.5^{\circ}$ $h = -7 \rightarrow 7$ $k = -24 \rightarrow 24$ $l = -22 \rightarrow 25$
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	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
F1	1.3085 (4)	0.41875 (10)	0.55088 (8)	0.1071 (7)	
01	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)	
03	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 $(Å^2)$

	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)
01	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)
03	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, °)

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)	С9—Н9А	0.970
C2—C3	1.460 (3)	С9—Н9В	0.970
С2—С7	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
С6—С7	1.479 (3)	C20—H20	0.930
С8—С9	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)		
F1C21	3,597 (3)	C1···H9B ⁱⁱ	3.3111
01···C1	2.832 (3)	C3···H6A ⁱⁱ	3,1946
01···C7	3523(3)	C3···H23C ⁱⁱ	3 5247
01···C14	3.194 (3)	C4···H6A ⁱⁱ	3.0348
02···C1	2.844(3)	C4···H23C ⁱⁱ	3 1830
02	3517(3)	C6···H4A ^{iv}	3 4001
02···C14	3 185(3)	$C6\cdots H20^{xi}$	3 5732
02 °C14 03…C1	2 900 (3)	$C8 \cdots H1^{iv}$	3 5015
C2···C5	2 919 (3)	$C8\cdots H18^{v}$	3 4780
C2···C8	2.519(3)	C9···H1 ^{iv}	3 3551
C2···C15	3,009 (3)	C11H23A ^{vi}	3 4709
C2C23	3 367 (3)	$C11 \cdots H23C^{vi}$	3 5698
C3···C6	2.918(4)	$C11 \cdots H24A^{xii}$	3 3105
C3…C14	2.910(4) 3.222(3)	$C12 \cdots H9B^{ii}$	3 3236
C3···C23	3.036(4)	$C12 \cdot H24C^{ii}$	3 2611
C4···C7	2 809 (4)	C13H9B ⁱⁱ	3 3720
C7…C13	2,755 (3)	C14···H17 ⁱⁱ	3 4730
C7…C14	3463(3)	$C14\cdots H22B^{iii}$	3 3846
C7C23	3.165(3) 3.144(3)	C15····H22C ^{vi}	3 3203
C8…C11	2 806 (3)	C15H25Bix	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)	$C16 \cdot H22C^{vi}$	3 0316
C10···C13	2.910(1)	C16···H25B ^{ix}	3 2531
C12···C14	3 142 (3)	$C17 \cdots H9A^{ix}$	3 0860
C12···C25	3,099(3)	C17···H21 ^{iv}	3 4376
C13···C15	3,203(3)	$C17 \cdot H22A^{vi}$	3 1996
C13····C25	3.203(3) 3.452(3)	C17 H22R $C17 H22C^{vi}$	3 5190
C14···C21	3,009 (3)	$C17 \cdots H24B^{ix}$	3 3980
C16···C19	2.761(3)	$C17 \cdots H25A^{i}$	3 2675
C17···C20	2.701(3) 2 771(4)	$C17 \cdot H25R^{i}$	3 5667
C18····C21	2.771(4) 2 754 (4)	$C17 \cdot H25B$ $C17 \cdot H14^{iv}$	3 54 (3)
F1C4 ⁱ	2.734(4) 3.474(3)	$C18 \cdots H9A^{ix}$	3 0056
F1···C6 ⁱ	3.77(3)	C18H21 ^{iv}	3 1224
$F1 \cdots C7^{i}$	3.512(3)	$C18 \cdots H22 \Delta^{vi}$	3.1224
0103 ⁱⁱ	3,535(3)	$C18 \cdots H25 \Delta^{i}$	3 1618
01···C23 ⁱⁱ	3,357(3) 3,494(4)	C19H9Aix	3 0437
02023	3,533 (4)	C19H20x	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
01…H4A	2.8387	C22···H14 ^{vii}	3.19 (3)
01…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
02…H1	2.6498	C23···H24B ^{ix}	3.3204
02H11A	2.8347	$C24\cdots H11B^{xii}$	3.3831
02H11B	2.4886	C24···H23A ^{xi}	3.2261
02···H25A	3 5198	$C24\cdots H23B^{xi}$	3 4164
02	3 02 (3)	$C24\cdots H24A^{xii}$	3 3320
03···H6A	2,4523	C24···H25A ^{iv}	3 3600
03···H6B	2.6557	C24···H25C ^{iv}	3 4827
03···H9A	2.0337	C25H17 ^v	3 2327
03H9B	2.1922	C_{25} ···H18 ^v	3 3155
03H15	3 31 (3)	C25H24B ⁱⁱ	3 3827
C1H15	2.51(3)	C_{25} H_{24} C_{12} H_{24} C_{12}	3 4616
C2H4A	2.03 (5)	H_{1}	3 5083
C2···H4B	2.9517		3.5015
C2H6A	3 1832		3 3 5 5 1
C2H6B	3.1052		2 5247
C2H23B	2 8304		2.3347
C2H14	2.0374		3.5555
C2H15	3.27(3)		2.5545
C2H1	2.70 (3)		2.0922
	2.0807		5.4001 2.4246
C21122.A	2.2002		2.4340
C2 U22D	2.014		5.4627 2.5917
C3	2.0914		5.581/ 2.1975
	5.59 (5) 2.2005		3.18/3
	3.3095		3.0419
C4H6B	2.7999		3.43//
C4···H22A	2.7237		3.0997
C4···H22B	2.6671	H4B···H23C ⁿ	2.5189
C4H22C	3.3330		3.2287
C4H23A	2.6551		3.0975
C4…H23B	2.6606		3.1946
C4···H23C	3.3172	H6A····C4 ^{IV}	3.0348
Со…Н4А	2.7173	H6A····H4A ¹ V	2.4346
C6···H4B	3.3234	$H6A \cdots H4B^{iv}$	3.0997

C6-H122A 2.6471 H6A-H20 ⁶¹ 3.5224 C6-H22B 3.3240 H6B-C10 ⁶¹ 3.5580 C6-H22C 2.6962 H6B-C20 ⁶¹ 3.5580 C6-H23A 3.3434 H6B-H20 ⁶¹ 3.2582 C6-H23B 2.6773 H9A-C16 ⁴¹ 3.2822 C6-H23C 2.7096 H9A-C17 ¹⁰ 3.0860 C7-H11 3.1660 H9A-C19 ¹¹ 3.0437 C7-H23B 2.8257 H9A-C20 ¹⁰ 3.1827 C7-H23C 3.5123 H9A-C11 ¹⁰ 3.637 C7-H13 3.04 (3) H9A-H11 ¹⁶¹ 3.5531 C8-H11A 3.1173 H9A-H11 ¹⁸¹ 3.5535 C8-H25A 2.8550 H9B-C1 ¹⁶¹ 3.2286 C9-H11A 2.7191 H9B-C1 ¹⁶¹ 3.3111 C8-H25A 2.850 H9B-C1 ¹⁶¹ 3.3226 C9-H11B 3.3179 H9B-H1 ¹⁶¹ 2.5347 C9-H24A 3.260 H9B-H25A ¹⁶¹ 3.270 C9-H24A 2.6682 H11A-H224 ¹⁶¹ 3.297				
C6-H22B 3.3240 H6BF1* 2.8599 C6-H22C 2.6962 H6BC20* 3.5350 C6-H23A 3.3434 H6BH20* 2.8574 C6-H23B 2.6773 H9AC16* 3.2382 C6-H23C 2.7096 H9AC17* 3.0860 C7-H1 3.1660 H9AC18* 3.005 C7-H13B 2.8257 H9AC20* 3.1827 C7-H23C 3.5123 H9AC21* 3.2544 C8-H11 3.1658 H9AH17* 3.5637 C8-H11 3.1658 H9AH17* 3.5637 C8-H13 3.1658 H9AH17* 3.5315 C8-H25A 2.8550 H9BC2* 3.0258 C8-H25A 2.8550 H9BC1* 3.111 C8-H15 3.40 (3) H9BC1* 3.3111 C8-H15 3.40 (3) H9BC1* 3.2276 C9-H11A 2.7191 H9BC12* 3.2287 C9-H24A 3.3260 H9BH1* 3.3720 C9-H25C <td>C6…H22A</td> <td>2.6471</td> <td>H6A····H20^{xi}</td> <td>3.5224</td>	C6…H22A	2.6471	H6A····H20 ^{xi}	3.5224
C6-H22C2.6962H6B-C20 ^a 3.5580C6-H23A3.3434H6B-H20 ^a 2.5574C6-H23C2.7096H9A-C17 ^a 3.2382C6-H23C2.7096H9A-C17 ^a 3.0860C7-H13.1660H9A-C17 ^a 3.0437C7-H23B2.8257H9A-C20 ^a 3.0437C7-H23B2.8257H9A-C20 ^a 3.0437C7-H23C3.5123H9A-C19 ^a 3.0437C7-H13C3.04(3)H9A-H18 ^a 3.5537C8-H113.1658H9A-H18 ^a 3.5553C8-H12A2.8550H9A-C1 ^a 3.0258C8-H15A3.40 (3)H9A-H18 ^a 3.3256C9-H11A2.7191H9B-C1 ^a 3.3270C9-H11B3.3179H9B-H1 ^b 2.5347C9-H24A3.3260H9B-H25A ^a 3.2878C9-H24B2.6728H11A-C2 ^a 3.2488C9-H25A2.6682H11A-C2 ^a 3.2970C9-H25B2.6957H11A-H22B ^a 3.2970C9-H25B2.6957H11A-H22B ^a 3.2970C9-H25A2.6849H11A-H22B ^a 3.2970C9-H25A2.6957H11A-H22B ^a 3.2970C9-H25A2.6957H11A-H22B ^a 3.2970C9-H25A2.6957H11A-H22B ^a 3.2970C9-H25A2.6957H11A-H22B ^a 3.2970C9-H25A2.6957H11A-H22B ^a 3.2970C9-H25A2.6957H11A-H22B ^a 3.2987C11-H9A3.3094H11A-H22B ^a 3.2987C11-H9A<	C6…H22B	3.3240	H6B…F1 ^v	2.8599
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6…H22C	2.6962	H6B····C20 ^{xi}	3.5580
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С6…Н23А	3.3434	H6B····H20 ^{xi}	2.8574
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С6…Н23В	2.6773	H9A…C16 ^{xi}	3.2382
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6…H23C	2.7096	H9A…C17 ^{xi}	3.0860
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С7…Н1	3.1660	H9A…C18 ^{xi}	3.0056
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С7…Н4А	3.1005	H9A…C19 ^{xi}	3.0437
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С7…Н23В	2.8257	H9A…C20 ^{xi}	3.1827
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7···H23C	3.5123	H9A····C21 ^{xi}	3.2544
C8H13.1658H9AH18*3.3955C8H11A3.1173H9AH18*3.3955C8H12A2.8550H9BC12*3.0258C8H25B3.5231H9BC12*3.3111C8H153.40 (3)H9BC12*3.3236C9H11A2.7191H9BC12*3.3236C9H11B3.3179H9BH25A*3.2878C9H24A3.3260H9BH25A*3.2878C9H24B2.6728H11AO2*3.3418C9H24B2.6728H11AC23*i3.1848C9H25A2.6682H11AH223*i3.2970C9H25B2.6957H11AH223*i3.2970C9H25C3.3375H11AH223*i2.5987C11H9A3.094H11AH234*i2.9027C11H9A3.3094H11AH23C*i2.9148C11H24A2.6947H11BC24*i3.3831C11H24B3.3354H11BH218*ii3.5508C11H24B3.352H11BH23A*i3.5428C11H24B3.352H11BH23C*i3.5355C11H25C2.6784H11BH23C*i3.5355C11H25C2.6784H11BH23C*i3.5428C11H25C2.6784H11BH23C*i3.5428C11H25C3.688H17C1**3.2402C12H143.31(3)H17H24*i3.5606C13H983.0200H17H24*i3.5506C13H983.0200H17H24*i3.5506C13H143.02(3)H17H24*i	С7…Н15	3.04 (3)	H9A…H17 ^{xi}	3.5637
C8H11A1.1173H9AH18 ^{sti} 3.4335C8H25A2.8550H9BO2 ^w 3.0258C8H25B3.5231H9BC1 ^w 3.3111C8H153.40 (3)H9BC12 ^w 3.3236C9H11A2.7191H9BC13 ^w 3.3720C9H11A2.7191H9BH1 ^w 2.5347C9H24A3.3260H9BH1 ^w 2.5347C9H24B2.6728H11AC23 ^{wi} 3.3418C9H24C2.6682H11AC23 ^{wi} 3.4184C9H25A2.6849H11AH22B ^{wi} 3.2970C9H25B2.6957H11AH22C ^{wi} 3.4992C9H25C3.3375H11AH22C ^{wi} 3.4992C9H25C3.3375H11AH22C ^{wi} 2.9148C11H9A3.3094H11AH22C ^{wi} 2.9148C11H9B2.7892H11AH22C ^{wi} 3.3831C11H24B3.3354H11BH11B ^{wim} 3.5508C11H24B3.33292H11BH23A ^{vi} 3.5428C11H25C2.6776H11BH23A ^{vi} 3.5428C11H25C2.6776H11BH24A ^{wim} 2.8592C12H112.7208H11BH24A ^{wim} 3.5355C12H143.31(3)H17C14 ^{wim} 3.5350C12H183.3065H17H24 ^{wim} 3.566C13H19A3.2125H17H124 ^{wim} 3.5606C13H143.02(3)H17H124 ^{wim} 3.5606C13H143.02(3)H17H124 ^{wim} 3.5506C13H143.02(3)H17H124 ^{wim} 3.5606 </td <td>C8…H1</td> <td>3.1658</td> <td>H9A···H18^v</td> <td>3,3955</td>	C8…H1	3.1658	H9A···H18 ^v	3,3955
C8-H25A2.8550H9B- $\cdot O2^n$ 3.0258C8-H25B3.5231H9B- $\cdot C1^{in}$ 3.3111C8-H153.40 (3)H9B- $\cdot C1^{in}$ 3.3111C9-H11A2.7191H9B- $\cdot C1^{in}$ 3.3236C9-H11B3.3179H9B- $\cdot H1^{in}$ 2.5347C9-H24A3.3260H9B- $\cdot H25A^{in}$ 3.2878C9-H24B2.6728H11A- $\cdot O2^{in}$ 3.3418C9-H25A2.6849H11A- $\cdot C23^{in}$ 3.1848C9-H25A2.6849H11A- $\cdot H22B^{in}$ 3.2970C9-H25B2.6957H11A- $\cdot H22B^{in}$ 3.2970C9-H25C3.3375H11A- $\cdot H22B^{in}$ 2.9987C11-H9A3.3094H11A- $\cdot H22C^{in}$ 3.4992C1-H9B2.7892H11A- $\cdot H22A^{ini}$ 2.9207C11-H24A2.6947H11B- $\cdot C24^{ini}$ 3.3831C11-H24B3.354H11B- $\cdot H11B^{inii}$ 3.5508C11-H24B3.3524H11B- $\cdot H24A^{ini}$ 2.8542C11-H25A2.6776H11B- $\cdot H24A^{ini}$ 2.8542C11-H25B3.3292H11B- $\cdot H24A^{ini}$ 2.8542C11-H25B3.3292H11B- $\cdot H24A^{ini}$ 3.8542C11-H25A2.6776H11B- $\cdot H24A^{ini}$ 3.8542C11-H25B3.3292H11B- $\cdot H24A^{ini}$ 3.8542C11-H25A2.6784H11B- $\cdot H24A^{ini}$ 3.8542C11-H25A2.6784H11B- $\cdot H24A^{ini}$ 3.85637C12-H143.31 (3)H17- $\cdot H24^{ini}$ 3.2402C12-H153.135H17- $\cdot C14^{ini}$ 3.240	C8…H11A	3.1173	H9A…H18 ^{xi}	3.4535
C8-H25B3.5231H9B-··C1*3.3111C8-·H25B3.5231H9B-··C1*3.3111C8-·H153.40 (3)H9B-··C12*3.3236C9-·H142.7191H9B-··C13*3.3720C9-·H183.3179H9B-··H1*2.5347C9-·H24A3.3260H9B-··H25A*3.2878C9-·H24B2.6728H11A···C2*3.3418C9-·H24C2.6682H11A···C2*3.3418C9-·H25A2.6849H11A···H22B*3.2970C9-·H25C3.3375H11A···H23A*2.5987C11-·H9A3.3094H11A···H23A*2.5987C11-·H9A3.3094H11A···H23A*2.9207C11-·H9B2.7892H11A···H24A**2.9207C11-·H24A2.6947H11B···C24**3.3831C11-·H24B3.3554H11B···H23A**3.5508C11-·H24B3.3529H11B··H23A**3.5508C11-·H24C2.6776H11B··H23A**3.5428C11-·H24C2.6776H11B··H23A**3.5428C11-·H25B3.3292H1B··H24C**3.5428C11-·H25C2.6776H11B··H23A**3.5508C11-·H25A2.6776H11B··H23A**3.5035C11-·H25A2.6776H11B··H23A**3.5428C11-·H25A2.6776H11B··H23A**3.5505C11-·H25A2.6776H11B··H23A**3.5428C11-·H25A2.6776H11B··H23A**3.5428C11-·H25A2.6776H11B··H23A**3.5637C12-·H163.3688H	C8H25A	2.8550	H9B····O2 ^{iv}	3.0258
C8H153.40 (3)H9B-··C12 ^{iv} 3.3236C9H11A2.7191H9B-··C13 ^{iv} 3.3720C9H11B3.3179H9B-··H11 ^{iv} 2.5347C9H24A3.2600H9B-··H25A ^{iv} 3.2878C9H24B2.6728H11A-··C23 ⁱⁱ 3.1848C9H24B2.6682H11A-··C23 ⁱⁱⁱ 3.1848C9H25A2.6682H11A-··H22B ^{iv} 3.2970C9H25B2.6957H11A-··H22C ⁱⁱⁱ 3.4992C9H25C3.3375H11A-··H23C ^{iv} 2.9148C11-··H9A3.3094H11A-··H23C ^{iv} 2.9148C11-··H9B2.7892H11A-··H23C ^{iv} 2.9148C11-··H9B2.7892H11A-··H23C ^{iv} 3.9831C11-··H24A2.6947H11B-··C24 ⁱⁱⁱ 3.3831C11-··H24B3.3354H11B-··H11B ^{iviii} 3.5508C11-··H24B3.3529H11B-··H23C ^{iv} 3.5355C11-··H25A2.6776H11B-··H23C ^{iv} 3.5355C11-··H25A2.6776H11B-··H24C ⁱⁱⁱ 3.5428C11-··H25A2.6776H11B-··H24C ⁱⁱⁱ 3.5428C11-··H25A2.6776H11B-··H24C ⁱⁱⁱ 3.5428C11-··H25A2.6776H11B-··H24C ⁱⁱⁱ 3.5428C11-··H25A2.6776H11B-··H24C ⁱⁱⁱ 3.5428C11-··H25A2.6774H11B-··H24C ⁱⁱⁱ 3.5428C11-··H25A2.6784H11B-··H24C ⁱⁱⁱ 3.1702C12-··H143.3165H17-··O14 ^{iv} 3.8695C12-··H153.1635H17-··O14 ^{iv} 3.8600C1	C8H25B	3.5231	H9B···C1 ^{iv}	3.3111
$C9 - H11A$ $C176(9)$ $H1B - C13^{in}$ 3.3720 $C9 - H11B$ 3.3179 $H9B - H1^{in}$ 2.5347 $C9 - H24A$ 3.3260 $H9B - H25A^{in}$ 3.2878 $C9 - H24B$ 2.6728 $H11A - C2^{in}$ 3.3418 $C9 - H24C$ 2.6682 $H11A - C2^{in}$ 3.1848 $C9 - H25A$ 2.6849 $H11A - H22B^{in}$ 3.2970 $C9 - H25A$ 2.6849 $H11A - H22B^{in}$ 3.2970 $C9 - H25B$ 2.6957 $H11A - H22A^{in}$ 2.5987 $C11 - H9A$ 3.3094 $H1A - H22A^{in}$ 2.9927 $C11 - H9B$ 2.7892 $H11A - H22A^{in}$ 2.9207 $C11 - H24A$ 2.6947 $H1B - C24^{ini}$ 3.3831 $C11 - H24A$ 2.6947 $H1B - H23A^{in}$ 3.5508 $C11 - H24A$ 2.6776 $H1B - H23A^{in}$ 3.5508 $C11 - H24B$ 3.3292 $H11B - H23A^{in}$ 3.5428 $C11 - H25C$ 2.6776 $H1B - H24C^{ini}$ 3.2402 $C11 - H25C$ 2.6784 $H1B - H24C^{ini}$ 3.2402 $C11 - H25C$ 2.6784 $H1B - H24C^{ini}$ 3.2402 $C12 - H1$ 2.7208 $H1B - H24C^{ini}$ 3.2402 $C12 - H25A$ 2.7712 $H17 - C1^{ini}$ 3.2327 $C12 - H25A$ 2.7712 $H17 - C14^{ini}$ 3.3260 $C13 - H9A$ 3.2000 $H17 - H24B^{ini}$ 3.5506 $C13 - H9A$ 3.2000 $H17 - H24B^{ini}$ 3.5506 $C13 - H1A$ 2.9274 $H17 - H24B^{ini}$ </td <td>C8H15</td> <td>3 40 (3)</td> <td>H9B····C12^{iv}</td> <td>3 3236</td>	C8H15	3 40 (3)	H9B····C12 ^{iv}	3 3236
C9H11BC13.17H12C13.17C9H12BC3.179H9BH12AC3.5347C9H24AC3.260H9BH25A ^{iv} C3.2878C9H24BC.6728H11AC23 ⁱⁱ C3.418C9H25AC.6682H11AH22B ⁱⁱ C3.2970C9H25BC.6957H11AH22B ⁱⁱ C3.2970C9H25BC.6957H11AH22C ⁱⁱ C4.992C9H25CC3.3375H11AH22C ⁱⁱ C9.987C11H9AC.7892H11AH24A ^{sii} C.9987C11H9BC.7892H11AH24A ^{sii} C.9207C11H24BC.6947H11BC24 ^{sii} C.3831C11H24BC.6776H11BH23A ^{si} C.5588C11H24BC.6776H11BH23C ^{si} C.5585C11H25DC.6776H11BH24C ^{sii} C.5542C11H25BC.20207H11BH24C ^{sii} C.5555C11H25BC.20208H11BH24C ^{sii} C.1722C12H1C.7208H11BH24C ^{sii} C.1722C12H1C.7208H11BH24C ^{sii} C.1722C12H25CC.4712H17C14 ^{sii} C.28952C12H25CC.4135H17C14 ^{sii} C.2322C12H14C.31(3)H17H24 ^{sii} C.28952C12H15C.125H17H24 ^{sii} C.28563C13H18C.3065H17H24 ^{sii} C.28561C13H18C.3065H17H24 ^{sii} C.28561C13H18C.3065H17H24 ^{sii} C.28564C13H18C.3016H17H24 ^{sii} <td< td=""><td>C9H11A</td><td>2 7191</td><td>H9B···C13^{iv}</td><td>3 3720</td></td<>	C9H11A	2 7191	H9B···C13 ^{iv}	3 3720
C9H24A3.3260H9BH25A ^{IV} 3.2878C9H24B2.6728H11A- \cdot -O2 ^{IV} 3.3418C9H24C2.6682H11A- \cdot -H22B ^{II} 3.2970C9H25A2.66849H11A- \cdot -H22B ^{II} 3.2970C9H25B2.6957H11A- \cdot -H22C ^{II} 3.4992C9H25C3.3375H11A- \cdot -H23A ^{II} 2.5987C11H9A3.3094H11A- \cdot -H23C ^{II} 2.9148C11H9B2.7892H11A- \cdot -H23A ^{III} 2.9207C11H24A2.6947H11B- \cdot C24 ^{III} 3.3831C11H24B3.3354H11B- \cdot H11B ^{IIII} 3.5508C11H24C2.6797H11B- \cdot H23A ^{III} 3.5428C11H25A2.6776H11B- \cdot H23C ^{III} 3.5355C11H25B3.3292H11B- \cdot H24A ^{III} 2.8542C11H25B3.3292H11B- \cdot H24C ^{III} 3.5428C11H25C2.6784H11B- \cdot H24C ^{III} 3.2402C12H12.7208H11B- \cdot H24C ^{III} 3.172C12H9B3.3688H17- \cdot O1 ^{IV} 2.8952C12H25C3.4135H17- \cdot C25 ^{III} 3.2360C13- \cdot H9A3.2125H17- \cdot H24 ^{III} 3.5637C13- \cdot H9B3.0000H17- \cdot H24B ^{III} 3.5666C13- \cdot H143.02(3)H17- \cdot H24B ^{III} 3.8860C13- \cdot H143.02(3)H17- \cdot H22A ^{III} 3.8876C13- \cdot H143.02(3)H17- \cdot H24B ^{III} 3.8876C13- \cdot H143.02(3)H17- \cdot H24B ^{III} 3.8876C13- \cdot H143.02(3)H17- \cdot H24B ^{III}	C9H11B	3 3179	H9B···H1 ^{iv}	2 5347
C9H24B2.6728H11AO2 ^w 3.3418C9H24C2.6682H11AO2 ^w 3.3418C9H25A2.6682H11AH22B ^{vi} 3.2970C9H25B2.6957H11AH22C ^{vi} 3.4992C9H25C3.3375H11AH22C ^{vi} 3.4992C11H9A3.3094H11AH22A ^{vii} 2.9148C11H9B2.7892H11AH24A ^{vii} 2.9207C11H24A2.6947H11BC24 ^{vii} 3.3831C11H24B3.3354H11BH11B ^{viii} 3.5508C11H24B3.3354H11BH24A ^{vii} 3.5428C11H24C2.6797H11BH23A ^{vi} 3.5428C11H25A2.6776H11BH24C ^{vii} 3.5355C11H25B3.3292H11BH24A ^{vii} 2.8542C11H25C2.6784H11BH24C ^{vii} 3.2402C12H12.7208H11BH24C ^{vii} 3.1172C12H9B3.3688H17O1 ^w 2.8952C12H25C3.4135H17C25 ^{vi} 3.2327C12H25C3.4135H17C25 ^{vi} 3.2327C12H143.31 (3)H17H24B ^{ix} 3.5663C13H9A3.2125H17H25A ⁱⁱ 2.8864C13H9A3.2125H17H25B ⁱ 2.8858C13H143.0065H17H25A ⁱⁱ 2.8858C13H143.02 (3)H17H25B ⁱ 2.8858C13H143.02 (3)H17H25B ⁱ 3.8858C13H143.02 (3)H17H14 ^{vi} 3.0895C14H212.7346H18C21 ^{vi} 3	C9H24A	3 3260	H9B···H25A ^{iv}	3 2878
C9H24C2.6682H11AC23 ^{si} 3.1848C9H25A2.6849H11AH22B ^{si} 3.2970C9H25B2.6957H11AH22C ^{si} 3.4992C9H25C3.3375H11AH22A ^{si} 2.5987C11H9A3.3094H11AH22A ^{si} 2.9148C11H9B2.7892H11AH24A ^{sii} 2.9207C11H24A2.6947H11BC24 ^{sii} 3.3831C11H24B3.3354H11BH11B ^{siii} 3.5508C11H24B3.3354H11BH11B ^{siii} 3.5508C11H24B3.3354H11BH24A ^{sii} 3.5428C11H25A2.6776H11BH24A ^{sii} 3.5428C11H25B3.3292H11BH24C ^{sii} 3.5355C11H25C2.6784H11BH24C ^{sii} 3.2402C12H12.7208H11BH24C ^{sii} 3.2402C12H12.7208H11BH24C ^{sii} 3.1172C12H9B3.3688H17C14 ^{iv} 3.8952C12H25A2.7712H17C14 ^{iv} 3.4730C12H25C3.4135H17C25 ⁱ 3.2327C12H143.31 (3)H17H24 ^{sii} 3.5637C13H9B3.0200H17H24 ^{sii} 3.5637C13H1B3.3065H17H25 ^{si} 2.8858C13H1B3.15 (3)H17H25 ^{si} 3.8858C13H143.02 (3)H17H25 ^{si} 3.8444C15H172.6261H18-·C21 ^{si} 3.4206C15H172.6261H18-·C21 ^{si} 3.4206C15H122.6687H18-·C21 ^{si}	C9H24B	2 6728	H11A····O2 ^{iv}	3 3418
C9H25A2.6849H11AH22B*i3.2970C9H25B2.6957H11AH22C*i3.4992C9H25C3.3375H11AH22A*i2.5987C11H9A3.3094H11AH23A*i2.9148C11H9B2.7892H11AH24A*ii2.9207C11H24B3.354H11BC24*ii3.3831C11H24B3.354H11BH118*iii3.5508C11H24B3.354H11BH123A*i3.5428C11H24B3.354H11BH213A*i3.5428C11H25A2.6776H11BH23A*i3.5428C11H25B3.3292H11BH24A*ii2.8542C11H25B3.3292H11BH24A*ii3.842C11H25C2.6784H11BH24C*ii3.2402C12H12.7208H11BH24C*ii3.1172C12H9B3.3688H17O1*2.8952C12H25A2.7712H17C14**3.4730C12H25C3.4135H17C25*i3.2327C12H143.31 (3)H17H24**3.506C13H9B3.0200H17H24**3.5506C13H1A2.9274H17H24**3.1705C13H1B3.3065H17H24**3.1705C13H1B3.02 (3)H17H25*2.8588C13H143.02 (3)H17H25*3.8895C13H153.15 (3)H17H25*3.4484C15H13.2578H18C2*3.4206C15H172.6261H18C21*3.1313	C9H24C	2.6682	H11A····C23 ^{vi}	3.1848
C9H25B 2.6957 H11AH22C ^{ij} 3.4992 C9H25C 3.3375 H11AH22C ^{ij} 2.5987 C11H9A 3.3094 H11AH23C ^{ij} 2.9148 C11H9B 2.7892 H11AH24A ^{xii} 2.9207 C11H24A 2.6947 H11BC24 ^{xii} 3.3831 C11H24B 3.3354 H11BH11B ^{xiiii} 3.5508 C11H24C 2.6797 H11BH23A ^{xij} 3.5556 C11H24C 2.6797 H11BH23A ^{xij} 3.5555 C11H25B 3.2922 H11BH24A ^{xiii} 2.8542 C11H25C 2.6784 H11BH24C ^{xii} 3.2402 C12H1 2.7208 H11BH24C ^{xii} 3.2402 C12H1 2.7208 H11BH24C ^{xii} 3.1172 C12H25A 2.7712 H17C14 ^{iv} 3.4730 C12H25A 2.7712 H17C25 ⁱ 3.2327 C12H25C 3.4135 H17H24A ^{xii} 3.5637 C13H9A 3.2125 H17H24B ^{ix} 3.5666 C13H1A 2.9274 H17H24B ^{ix} 3.1705 C13H1B 3.065 H17H25A ⁱ 2.8640 C13H1B $3.02(3)$ H17H25B ⁱ 2.8858 C13H14 $3.02(3)$ H17H25B ⁱ 3.8895 C13H14 $3.02(3)$ H17H25C ⁱ 3.44780 C13H14 $3.02(3)$ H17H25C ⁱ 3.44780 C13H14 $3.02(3)$ H17H25C ⁱ 3.44780 C13H14 3.2578 H18C3 ⁱ 3.4484 C15H17 2.6261 <td>C9H25A</td> <td>2 6849</td> <td>H11A···H22B^{vi}</td> <td>3 2970</td>	C9H25A	2 6849	H11A···H22B ^{vi}	3 2970
ConstructConstructConstructConstructConstruct 3.375 H11AH23A^{vi} 2.5987 C11H9A 3.3094 H11AH23A^{vi} 2.5987 C11H9B 2.7892 H11AH23A^{vi} 2.9207 C11H24A 2.6947 H11BC24x ⁱⁱⁱ 3.3831 C11H24B 3.3354 H11BH11B ^{siiii} 3.5508 C11H24C 2.6797 H11BH23A ^{vi} 3.5428 C11H24C 2.6776 H11BH23C ^{vi} 3.5355 C11H25B 3.3292 H11BH24C ^{vii} 3.2402 C12H1 2.7208 H11BH24C ^{viii} 3.2402 C12H1 2.7208 H11BH24C ^{viii} 3.2402 C12H9B 3.3688 H17O1 ^{iv} 2.8952 C12H25A 2.7712 H17C25 ⁱ 3.2327 C12H14 $3.31(3)$ H17H9A ^{ix} 3.5637 C13H9A 3.2125 H17H24 ^{iv} 3.3260 C13H9B 3.0000 H17H24 ^{iv} 3.3260 C13H1A 2.9274 H17H24 ^{iv} 3.3260 C13H1B 3.3065 H17H25A ⁱ 2.8858 C13H1B $3.02(3)$ H17H25B ⁱ 2.8858 C13H1B $3.15(3)$ H17H25B ⁱ 2.8858 C13H14 $3.15(3)$ H17H14 ^{iv} 3.0895 C13H15 $3.15(3)$ H17H25C ⁱ 3.4760 C13H14 2.6261 H18C20 ^{iv} 3.4206 C15H17 2.6261 H18C20 ^{iv} 3.4206 C15H12 2.6687 H18-	C9H25B	2.6957	H11A···H22C ^{vi}	3 4992
C11H9A3.3094H11AH23Cvi2.9148C11H9B2.7892H11AH24Asii2.9207C11H24A2.6947H11BC24sii3.3831C11H24B3.3354H11BH11Bsiii3.5508C11H24B3.3354H11BH123Asii3.5508C11H24B3.3354H11BH23Asii3.5428C11H25A2.6776H11BH23Csii3.5355C11H25B3.3292H11BH24Asii2.8542C11H25B3.3292H11BH24Cii3.2402C12H12.7208H11BH24Cii3.2402C12H12.7208H11BH24Ciii3.1172C12H9B3.3688H17O14iv2.8952C12H25A2.7712H17C14iv3.4730C12H25A2.7712H17C25i3.2327C12H25A3.4135H17H9Aix3.5637C13H9A3.2125H17H21iv3.3260C13H9A3.2125H17H24Bix3.1705C13H1A2.9274H17H24Bix3.1705C13H1B3.3065H17H25Ai2.8640C13H1B3.02(3)H17H25Bi2.8858C13H143.02 (3)H17H25Ci3.44786C13H153.15 (3)H17H25Ci3.4484C15H13.2578H18C8i3.4484C15H172.6261H18C20iv3.4206C15H212.6687H18C20iv3.4313	C9H25C	3 3375	H11A···H23A ^{vi}	2 5987
C11H9B2.7892H11AH2C2.9207C11H9B2.7892H11AH2C4X ^{sii} 2.9207C11H24A2.6947H1BC24 ^{sii} 3.3831C11H24B3.3354H11BH11B ^{stiii} 3.5508C11H24C2.6797H11BH21A ^{stii} 3.5428C11H25A2.6776H11BH23A ^{sii} 3.5428C11H25B3.3292H11BH24A ^{stii} 2.8542C11H25B3.3292H11BH24C ^{sii} 3.2402C12H12.7208H11BH24C ^{sii} 3.1172C12H9B3.3688H17O1 ^{iv} 2.8952C12H25A2.7712H17C14 ^{iv} 3.4730C12H25A2.7712H17C14 ^{iv} 3.4730C12H25C3.4135H17H21 ^{iv} 3.3260C13H9A3.2125H17H24 ^{sii} 3.5506C13H9A3.0200H17H24 ^{sii} 3.5506C13H1A2.9274H17H24 ^{sii} 3.1705C13H1B3.3065H17H25A ⁱⁱ 2.8640C13H1B3.02(3)H17H25B ⁱⁱ 2.8858C13H143.02 (3)H17H25B ⁱⁱ 3.4858C13H153.15 (3)H17H14 ^{iv} 3.0895C14H212.7346H18O3 ⁱⁱ 3.4484C15H13.2578H18C20 ^{iv} 3.4206C15H212.6687H18C20 ^{iv} 3.4206	C11H9A	3,3094	H11A···H23C ^{vi}	2.9148
C11H24AC.6947H11B···C24*ii3.3831C11H24B3.3354H11B···H11B*iii3.5508C11H24B2.6797H11B···H11B*iii3.5508C11H24C2.6776H11B···H23A*i3.5428C11H25A2.6776H11B···H23C*i3.5355C11H25B3.3292H11B···H24A*ii2.8542C11H25C2.6784H11B···H24C*i3.2402C12H12.7208H11B···H24C*i3.1172C12H9B3.3688H17O1*2.8952C12H25A2.7712H17C14*3.4730C12H25C3.4135H17C25*3.2327C12H143.31 (3)H17H9A*3.5637C13H9A3.2125H17H21*3.3260C13H9B3.0200H17H22**i3.5506C13H11A2.9274H17H24*3.1705C13H183.3065H17H25*2.8858C13H183.02 (3)H17H25*2.8858C13H143.02 (3)H17H25*3.445*6C13H153.15 (3)H17H25*3.4484C15H13.2578H18···C20*3.4484C15H12.6261H18···C20*3.4206C15H212.6687H18···C20*3.4206	C11H9B	2.7892	H11A…H24A ^{xii}	2.9207
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11H24A	2,6947	H11B····C24 ^{xii}	3 3831
C11 \cdots H24C2.6797H1B \cdots H23A*i3.5428C11 \cdots H25A2.6776H1B \cdots H23C*i3.5355C11 \cdots H25B3.3292H1B \cdots H24A*ii2.8542C11 \cdots H25C2.6784H1B \cdots H24C*ii3.2402C12 \cdots H12.7208H1B \cdots H24C*ii3.1172C12 \cdots H9B3.3688H17 \cdots O1*v2.8952C12 \cdots H25A2.7712H17 \cdots C14*v3.4730C12 \cdots H25A2.7712H17 \cdots C14*v3.4730C12 \cdots H25A3.2125H17 \cdots H21*v3.260C13 \cdots H9A3.2125H17 \cdots H21*v3.3260C13 \cdots H9B3.0200H17 \cdots H24*s3.5506C13 \cdots H1B3.3065H17 \cdots H24*s3.1705C13 \cdots H1B3.3065H17 \cdots H25A*i2.8640C13 \cdots H1B3.02 (3)H17 \cdots H25B*i2.8858C13 \cdots H143.02 (3)H17 \cdots H25B*i2.8858C13 \cdots H143.02 (3)H17 \cdots H25B*i3.4484C15 \cdots H13.2578H18 \cdots C3*i3.4484C15 \cdots H172.6261H18 \cdots C20*v3.4206C15 \cdots H172.6261H18 \cdots C20*v3.4206C15 \cdots H212.6687H18 \cdots C21*v3.1313	C11H24B	3 3354	H11B····H11B ^{xiii}	3 5508
C11 ···H25A2.6776H11B ···H23C ^{vi} 3.5355C11 ···H25B3.3292H11B ···H24A ^{xii} 2.8542C11 ···H25C2.6784H11B ···H24C ⁱⁱ 3.2402C12 ···H12.7208H11B ···H24C ^{xii} 3.1172C12 ···H9B3.3688H17···O1 ^{iv} 2.8952C12 ···H9B3.3688H17···C14 ^{iv} 3.4730C12 ···H25A2.7712H17···C14 ^{iv} 3.4730C12 ···H25C3.4135H17···C25 ⁱ 3.2327C12 ···H43.31 (3)H17···H9A ^{ix} 3.5637C13 ···H9A3.2125H17···H21 ^{iv} 3.3260C13 ···H9B3.0200H17···H24B ^{ix} 3.1705C13 ···H1A2.9274H17···H24B ^{ix} 3.1705C13 ···H1B3.3065H17···H25A ⁱ 2.8640C13 ···H143.02 (3)H17···H25B ⁱ 2.8588C13 ···H143.02 (3)H17···H25C ⁱ 3.4576C13 ···H143.02 (3)H17···H25C ⁱ 3.4576C13 ···H143.2578H18···C20 ^{iv} 3.4484C15 ···H172.6261H18···C20 ^{iv} 3.4206C15 ···H212.6687H18···C21 ^{iv} 3.1313	C11H24C	2.6797	H11B····H23A ^{vi}	3.5428
C11 ···H25B 3.3292 H11B···H24A ^{xii} 2.8542 C11 ···H25C 2.6784 H11B···H24C ⁱⁱⁱ 3.2402 C12···H1 2.7208 H11B···H24C ⁱⁱⁱ 3.2402 C12···H9B 3.3688 H11B···H24C ^{xiii} 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···H24B ^{ix} 3.1705 C13···H1A 2.9274 H17···H24B ^{ix} 3.1705 C13···H1B 3.3065 H17···H25A ⁱ 2.8640 C13···H18 3.02 (3) H17···H25B ⁱ 2.858 C13···H14 3.02 (3) H17···H25D ⁱ 3.4576 C13···H15 3.15 (3) H17···H25D ⁱ 3.4576 C13···H14 3.02 (3) H17···H25D ⁱ 3.4576 C13···H14 3.02 (3) H17···H45B ⁱ 3.4576 <	C11H25A	2.6776	H11B····H23C ^{vi}	3.5355
C11 \cdots H25C2.6784H11B \cdots H24C ⁱⁱ 3.2402C12 \cdots H12.7208H11B \cdots H24C ⁱⁱ 3.1172C12 \cdots H9B3.3688H17 \cdots O1 ^{iv} 2.8952C12 \cdots H25A2.7712H17 \cdots C14 ^{iv} 3.4730C12 \cdots H25C3.4135H17 \cdots C25 ⁱ 3.2327C12 \cdots H143.31 (3)H17 \cdots H9A ^{ix} 3.5637C13 \cdots H9A3.2125H17 \cdots H21 ^{iv} 3.3260C13 \cdots H9B3.0200H17 \cdots H22A ^{vi} 3.5506C13 \cdots H1B3.3065H17 \cdots H25A ⁱ 2.8640C13 \cdots H1B3.3065H17 \cdots H25B ⁱ 2.8858C13 \cdots H143.02 (3)H17 \cdots H25B ⁱ 2.8858C13 \cdots H143.02 (3)H17 \cdots H25B ⁱ 3.4576C13 \cdots H153.15 (3)H17 \cdots H25C ⁱ 3.4576C13 \cdots H143.02 (3)H17 \cdots H25B ⁱ 3.895C14 \cdots H212.7346H18 \cdots O3 ⁱ 3.4484C15 \cdots H13.2578H18 \cdots C8 ⁱ 3.4780C15 \cdots H172.6261H18 \cdots C20 ^{iv} 3.4206C15 \cdots H212.6687H18 \cdots C21 ^{iv} 3.1313	C11H25B	3 3292	H11B···H24A ^{xii}	2.8542
C11D12D13D13D13C12H12.7208H11BH124Cxii3.1172C12H19B3.3688H17C10iv2.8952C12H25A2.7712H17C14iv3.4730C12H25C3.4135H17C25i3.2327C12H143.31 (3)H17H17H18C13H9A3.2125H17H17H24CxiiC13H9B3.0200H17H24Cxii3.5667C13H183.0200H17H24Cxii3.5066C13H183.0655H17H24Bix3.1705C13H183.3065H17H25Ai2.8640C13H25A2.9519H17H25Bi2.8858C13H143.02 (3)H17H25Ci3.4576C13H153.15 (3)H17H183.0895C14H212.7346H183.47803.4780C15H172.6261H18H183.4206C15H172.6261H18H183.4206C15H173.2578H18H183.4206C15H172.6261H18H183.4206C15H172.6261H18H183.4206C15H212.6687H18H213.1313	C11H25C	2.6784	H11B···H24C ⁱⁱ	3.2402
C12···H9B3.3688H17···O1 ^{iv} 2.8952C12···H25A2.7712H17···C14 ^{iv} 3.4730C12···H25C3.4135H17···C25 ⁱ 3.2327C12···H143.31 (3)H17···H9A ^{ix} 3.5637C13···H9A3.2125H17···H21 ^{iv} 3.3260C13···H9B3.0200H17···H22A ^{vi} 3.5506C13···H1A2.9274H17···H24B ^{ix} 3.1705C13···H1B3.3065H17···H25A ⁱ 2.8640C13···H1B3.02 (3)H17···H25B ⁱ 2.8858C13···H143.02 (3)H17···H25C ⁱ 3.4576C13···H153.15 (3)H17···H14 ^{iv} 3.0895C14···H212.7346H18···O3 ⁱ 3.4484C15···H13.2578H18···C8 ⁱ 3.4780C15···H172.6261H18···C21 ^{iv} 3.1313	C12…H1	2.7208	H11B···H24C ^{xii}	3.1172
C12 \cdot H25A2.7712H17 \cdot C14 ^{iv} 3.4730C12 \cdot H25C3.4135H17 \cdot C25 ⁱ 3.2327C12 \cdot H143.31 (3)H17 \cdot H9A ^{ix} 3.5637C13 \cdot H9A3.2125H17 \cdot H21 ^{iv} 3.3260C13 \cdot H9B3.0200H17 \cdot H22A ^{vi} 3.5506C13 \cdot H1A2.9274H17 \cdot H24B ^{ix} 3.1705C13 \cdot H1B3.3065H17 \cdot H25A ⁱ 2.8640C13 \cdot H1B3.02 (3)H17 \cdot H25B ⁱ 2.8858C13 \cdot H143.02 (3)H17 \cdot H25C ⁱ 3.4576C13 \cdot H153.15 (3)H17 \cdot H26C ⁱ 3.4576C13 \cdot H172.7346H18 \cdot C3 ⁱ 3.4484C15 \cdot H13.2578H18 \cdot C20 ^{iv} 3.4206C15 \cdot H212.6687H18 \cdot C21 ^{iv} 3.1313	C12···H9B	3 3688	H17····O1 ^{iv}	2.8952
C12 H25C 3.4135 $H17 \cdots C25^i$ 3.2327 C12 \cdots H14 $3.31 (3)$ $H17 \cdots H9A^{ix}$ 3.5637 C13 \cdots H9A 3.2125 $H17 \cdots H21^{iv}$ 3.3260 C13 \cdots H9B 3.0200 $H17 \cdots H22A^{vi}$ 3.5506 C13 \cdots H11A 2.9274 $H17 \cdots H24B^{ix}$ 3.1705 C13 \cdots H11B 3.3065 $H17 \cdots H25A^i$ 2.8640 C13 \cdots H18 $3.02 (3)$ $H17 \cdots H25B^i$ 2.8858 C13 \cdots H14 $3.02 (3)$ $H17 \cdots H25B^i$ 2.8858 C13 \cdots H15 $3.15 (3)$ $H17 \cdots H25C^i$ 3.4576 C13 \cdots H15 $3.15 (3)$ $H17 \cdots H25C^i$ 3.4484 C15 \cdots H1 3.2578 $H18 \cdots C3^i$ 3.4780 C15 \cdots H17 2.6261 $H18 \cdots C20^{iv}$ 3.4206 C15 \cdots H21 2.6687 $H18 \cdots C21^{iv}$ 3.1313	C12···H25A	2 7712	$H17C14^{iv}$	3 4730
C12 \cdots H143.31 (3)H17 \cdots H9A ^{ix} 3.5637C13 \cdots H9A3.2125H17 \cdots H21 ^{iv} 3.3260C13 \cdots H9B3.0200H17 \cdots H22A ^{vi} 3.5506C13 \cdots H1A2.9274H17 \cdots H24B ^{ix} 3.1705C13 \cdots H1B3.3065H17 \cdots H25A ⁱ 2.8640C13 \cdots H1B3.02 (3)H17 \cdots H25B ⁱ 2.8858C13 \cdots H143.02 (3)H17 \cdots H25C ⁱ 3.4576C13 \cdots H153.15 (3)H17 \cdots H25C ⁱ 3.4576C13 \cdots H172.7346H18 \cdots O3 ⁱ 3.4484C15 \cdots H13.2578H18 \cdots C8 ⁱ 3.4780C15 \cdots H172.6261H18 \cdots C21 ^{iv} 3.1313	C12···H25C	3.4135	$H17C25^{i}$	3.2327
C12H11 $3.010(9)$ H11 1.011 C13H17H11H11 3.260 C13H17H12 1.011 3.3260 C13H18 3.0200 H17 $H17$ $H124^{vi}$ C13H1A 2.9274 H17 $H124B^{ix}$ 3.1705 C13H1B 3.3065 H17 $H125A^i$ 2.8640 C13H1B $3.02(3)$ H17 $H125B^i$ 2.8858 C13H14 $3.02(3)$ H17 $H125C^i$ 3.4576 C13H15 $3.15(3)$ H17 $H14^{iv}$ 3.0895 C14H21 2.7346 H18 $O3^i$ 3.4484 C15H17 2.6261 H18 $C20^{iv}$ 3.4206 C15H17 2.6687 H18 $C21^{iv}$ 3.1313	C12···H14	3 31 (3)	H17···H9A ^{ix}	3 5637
C13 ···H9B 3.0200 H17 ···H21 3.5506 C13 ···H1A 2.9274 H17 ···H22A ^{vi} 3.5506 C13 ···H1B 3.3065 H17 ···H24B ^{ix} 3.1705 C13 ···H1B 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 ···H25C ⁱ 3.4576 C13 ···H15 3.15 (3) H17 ···H25C 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	С13…Н9А	3 2125	H17···H21 ^{iv}	3 3260
C13 ···H11A 2.9274 H17 ···H22H 3.1705 C13 ···H11B 3.3065 H17 ···H24B ^{ix} 3.1705 C13 ···H1B 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 ···H25C ⁱ 3.4576 C13 ···H15 3.15 (3) H17 ···H14 ^{iv} 3.0895 C14 ···H21 2.7346 H18 ···C3 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	C13···H9B	3 0200	H17···H22A ^{vi}	3 5506
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	C13···H11A	2.9274	H17···H24B ^{ix}	3.1705
C13 ··· H25A 2.9519 H17 ··· H25B ⁱ 2.8858 C13 ··· H14 3.02 (3) H17 ··· H25B 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	C13…H11B	3,3065	H17···H25A ⁱ	2.8640
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···C3 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	C13H25A	2.9519	H17···H25B ⁱ	2.8858
C13···H15 3.15 (3) H17···H14 ^{iv} 3.0895 C14···H21 2.7346 H18···C3 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	C13···H14	3.02 (3)	H17···H25C ⁱ	3.4576
C14···H21 2.7346 H17··III1 3.0000 C15···H1 3.2578 H18···C8 ⁱ 3.4484 C15···H17 2.6261 H18···C20 ^{iv} 3.4206 C15···H21 2.6687 H18···C21 ^{iv} 3.1313	С13…Н15	3.15 (3)	H17···H14 ^{iv}	3.0895
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	C14…H21	2.7346	H18····O3 ⁱ	3.4484
C15···H17 2.6261 H18···C20 ^{iv} 3.4206 C15···H21 2.6687 H18···C21 ^{iv} 3.1313	C15H1	3.2578	H18····C8 ⁱ	3.4780
C15···H21 2.6687 H18···C21 ^{iv} 3.1313	C15…H17	2.6261	H18····C20 ^{iv}	3.4206
	C15…H21	2.6687	H18····C21 ^{iv}	3.1313

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 [×]	3.0448
C19…H21	3,1964	H20····O3 ^{ix}	3.5868
C20H18	3.2361	H20····C6 ^{ix}	3.5732
C21H17	3.2251	H20C19 ^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	H_{20} , H_{20}	2 6610
C22H6B	2.5677	$H_{20} = H_{20}$ $H_{21} = C_{17}$	3 4376
C22H23A	2.5077	$H21C18^{ii}$	3.1224
C22 H23A	3 3055	$H21C22^{iii}$	3.5200
C22H23C	2.5055		2 1827
C22H4A	2.0427	H21H17ii	3.4027
C23H4R	2.6184	H21H18 ⁱⁱ	2.5200
C22	2.0104		2.7020
C22	2.3930		2.7508
С23Н22А	2.2112		5.4/51 2.2746
C23····H22A	5.5115 2.6714		3.3/40
С25…H22В	2.0/14		3.3408
C23····H22C	2.6239		3.1996
C24H9A	2.7833		3.3064
C24···H9B	2.5485		3.5298
C24···HIIA	2.6092	H22A····C21 ^{vin}	3.5814
C24···HIIB	2.7298		3.5506
C24…H25A	3.3190	H22A···H21 ^{vn}	2.7368
C24…H25B	2.6590	H22A···H14 ^{vn}	2.9242
C24…H25C	2.6697	H22B····O2 ^{vn}	2.6029
С25…Н9А	2.5878	H22B····C14 ^{vn}	3.3846
С25…Н9В	3.3230	H22B···H1 ^{vn}	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
Н4А…Н23А	3.5130	H23A…O2 ^{vii}	3.2088

Н4А…Н23В	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
Н6А…Н22А	3.0515	H23B…O1 ^{iv}	3.0772
H6A…H22C	2.6270	H23B····C24 ^{ix}	3.4164
Н6А…Н23А	3.4987	H23B····H24A ^{ix}	3.0844
Н6А…Н23В	2.7933	H23B····H24B ^{ix}	2.8856
Н6А…Н23С	2.4373	H23B····H25B ^{ix}	3.2722
H6B…H22A	2.3597	H23B···H25C ^{ix}	3.4810
Н6В…Н22В	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	$H24A\cdots C11^{xii}$	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	$H24A\cdots H24C^{xii}$	3.0825
H11B…H24B	3.5944	$H24B\cdots C17^{xi}$	3,3980
H11B···H24C	3 0192	$H24B\cdots C23^{xi}$	3 3204
H11B…H25A	2.8774	$H24B\cdots C25^{iv}$	3.3827
H11B…H25B	3.5111	$H24B\cdots H17^{xi}$	3,1705
H11B…H25C	2 4423	$H24B\cdots H23A^{xi}$	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	$H24C\cdots C25^{iv}$	3.4616
H22B···H23A	2,5079	$H24C\cdots H11B^{iv}$	3 2402
H22B···H23B	3.5474	H24C···H11B ^{xii}	3.1172
H22B…H23C	2.9393	H24C···H24A ^{xii}	3.0825

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H22C…H23A	2.9083	H24C····H25A ^{iv}	2.9694
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H22C…H23B	3.4988	H24C···H25C ^{iv}	3.1036
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H22C…H23C	2.4290	H25A…C17 ^v	3.2675
$H24A \cdots H25A$ 3.5416 $H25A \cdots C24^{ii}$ 3.3600 $H24A \cdots H25B$ 2.9248 $H25A \cdots H26^{iii}$ 3.2878 $H24A \cdots H25C$ 2.4867 $H25A \cdots H17^{\circ}$ 2.8640 $H24B \cdots H25C$ 2.94867 $H25A \cdots H18^{iv}$ 2.6772 $H24B \cdots H25B$ 2.4823 $H25A \cdots H24C^{iii}$ 2.9694 $H24C \cdots H25C$ 2.9505 $H25A \cdots H24C^{iii}$ 3.5309 $H24C \cdots H25C$ 3.5428 $H25B \cdots C15^{iii}$ 3.509 $H24C \cdots H25C$ 3.5428 $H25B \cdots C16^{iii}$ 3.2531 $F1 \cdots H6A^{ii}$ 2.2877 $H25B \cdots C16^{iii}$ 3.5667 $F1 \cdots H6A^{ii}$ 3.2287 $H25B \cdots C17^{ii}$ 3.5667 $F1 \cdots H6A^{ii}$ 3.2287 $H25B \cdots H17^{\circ}$ 3.8663 $F1 \cdots H6A^{ii}$ 3.0975 $H25B \cdots H18^{iii}$ 3.1027 $O1 \cdots H25C^{iii}$ 3.0534 $H25C \cdots C1^{iii}$ 3.5911 $O1 \cdots H23B^{iii}$ 3.0534 $H25C \cdots H23B^{iii}$ 3.2102 $O1 \cdots H23B^{iii}$ 3.0534 $H25C \cdots H23A^{iiii}$ 3.0227 $O2 \cdots H23B^{iii}$ 3.0534 $H25C \cdots H23A^{iiii}$ 3.0227 $O2 \cdots H23B^{iiii}$ 3.0419 $H25C \cdots H23B^{iiii}$ 3.0227 $O2 \cdots H23B^{iiii}$ 3.0419 $H25C \cdots H24B^{iiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiii$	H23B…H15	2.7912	H25A…C18 ^v	3.1618
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H24A…H25A	3.5416	H25A…C24 ⁱⁱ	3.3600
$H24A \cdots H25C$ 2.4867 $H25A \cdots H17^{\vee}$ 2.8640 $H24B \cdots H25A$ 3.5415 $H25A \cdots H24B^{``}$ 2.6772 $H24B \cdots H25B$ 2.4823 $H25A \cdots H24B^{``}$ 2.8715 $H24B \cdots H25C$ 2.9505 $H25A \cdots H24C^{``}$ 2.9694 $H24C \cdots H25B$ 3.5378 $H25B \cdots C15^{``}$ 3.5309 $H24C \cdots H25C$ 3.5428 $H25B \cdots C15^{``}$ 3.5309 $H24C \cdots H25C$ 3.5428 $H25B \cdots C15^{``}$ 3.2531 $F1 \cdots H6A^{``}$ 3.2287 $H25B \cdots C17^{``}$ 3.5667 $F1 \cdots H6A^{``}$ 3.2287 $H25B \cdots C17^{``}$ 3.5667 $F1 \cdots H6A^{``}$ 3.2287 $H25B \cdots H17^{``}$ 3.8858 $F1 \cdots H6A^{``}$ 3.0975 $H25B \cdots H17^{``}$ 3.8858 $F1 \cdots H20^{``}$ 3.0448 $H25B \cdots H17^{``}$ 3.4812 $O1 \cdots H23B^{``}$ 3.0772 $H25C \cdots C24^{``}$ 3.5911 $O1 \cdots H23B^{``}$ 3.0534 $H25C \cdots H17^{``}$ 3.4576 $O1 \cdots H23C^{``}$ 3.5911 $H25C \cdots H23B^{``}$ 3.0227 $O2 \cdots H23B^{``}$ 3.5911 $H25C \cdots H23B^{``}$ 3.0227 $O2 \cdots H4B^{```}$ 3.0419 $H25C \cdots H24B^{```}$ 3.0480 $O2 \cdots H23A^{```}$ 3.0419 $H25C \cdots H24B^{```}$ 3.0485 $O2 \cdots H11A^{```}$ 3.3418 $H14 \cdots C17^{```}$ $3.54(3)$ $O2 \cdots H14B^{```}$ 3.0288 $H4 \cdots H17^{```}$ 3.5369 $O2 \cdots H24B^{```}$ 3.0288 $H14 \cdots H22A^{```}$ 2.9242 $O2 \cdots H24B^{```}$ 3.0288 $H14 \cdots H22A^{```}$ <t< td=""><td>H24A…H25B</td><td>2.9248</td><td>H25A…H9Bⁱⁱ</td><td>3.2878</td></t<>	H24A…H25B	2.9248	H25A…H9B ⁱⁱ	3.2878
$H24B\cdots H25A$ 3.5415 $H25A\cdots H18^{v}$ 2.6772 $H24B\cdots H25B$ 2.4823 $H25A\cdots H24B^{in}$ 2.8715 $H24B\cdots H25C$ 2.9505 $H25A\cdots H24C^{in}$ 2.9694 $H24C\cdots H25B$ 3.5378 $H25B\cdots O1^{in}$ 3.5309 $H24C\cdots H25B$ 3.5378 $H25B\cdots O1^{in}$ 3.5106 $H14\cdots H15$ 2.71 (4) $H25B\cdots C15^{in}$ 3.3106 $H14\cdots H15$ 2.71 (4) $H25B\cdots C16^{in}$ 3.2531 $F1\cdots H6A^{in}$ 3.2287 $H25B\cdots C17^{in}$ 3.5667 $F1\cdots H6B^{in}$ 2.8599 $H25B\cdots H17^{in}$ 2.8858 $F1\cdots H20^{in}$ 3.0448 $H25B\cdots H18^{in}$ 3.1027 $O1\cdots H6A^{in}$ 3.0975 $H25B\cdots H23B^{in}$ 3.2722 $O1\cdots H16^{in}$ 3.0975 $H25B\cdots H123B^{in}$ 3.2722 $O1\cdots H17^{in}$ 2.8952 $H25C\cdots H24B^{in}$ 3.5911 $O1\cdots H23D^{in}$ 3.0772 $H25C\cdots H27^{in}$ 3.4576 $O1\cdots H23C^{in}$ 3.5309 $H25C\cdots H24B^{in}$ 3.2102 $O1\cdots H25C^{in}$ 3.5911 $H25C\cdots H24B^{in}$ 3.0202 $O2\cdots H24B^{in}$ 3.0419 $H25C\cdots H24B^{in}$ 3.0227 $O2\cdots H4B^{in}$ 3.0419 $H25C\cdots H24B^{in}$ 3.036 $O2\cdots H24B^{in}$ 3.0208 $H14\cdots H17^{in}$ 3.0895 $O2\cdots H24B^{in}$ 3.0208 $H14\cdots H17^{in}$ 3.0895 $O2\cdots H24B^{in}$ 3.0208 $H14\cdots H22A^{ini}$ 2.9242 $O2=H242C^{in}$ 2.8628 $H14\cdots H22A^{in}$ 2.9242 $O2=H242C^{in}$ 2.8	H24A…H25C	2.4867	H25A…H17 ^v	2.8640
H24B···H25B2.4823H25A···H24B ⁱⁱ 2.8715H24B···H25C2.9505H25A···H24C ⁱⁱ 2.9694H24C···H25B3.5378H25B···O1 ^{ai} 3.5309H24C···H25C3.5428H25B···C16 ^{ai} 3.2531F1···H4A ⁱ 2.6922H25B···C17 ⁱⁱ 3.5667F1···H6B ⁱⁱ 2.8599H25B···C17 ⁱⁱ 3.5623F1···H6B ⁱⁱ 2.8599H25B···C17 ⁱⁱ 3.5623F1···H6B ⁱⁱ 2.8599H25B···H18 ⁱⁱ 3.1027O1···H6A ⁱⁱ 3.0975H25B···H23B···H18 ⁱⁱ 3.2722O1···H17 ⁱⁱ 2.8952H25C···O1 ^{aii} 3.5911O1···H23B ⁱⁱ 3.0772H25C···C24 ⁱⁱ 3.4827O1···H23B ⁱⁱ 3.0772H25C···C14 ⁱⁱ 3.4911O1···H23B ⁱⁱ 3.0534H25C···H24B ⁱⁱⁱ 3.2012O1···H23B ⁱⁱ 3.509H25C···H24B ⁱⁱⁱ 3.2027O2···H4B ⁱⁱⁱ 3.0258H14···C17 ⁱⁱⁱ 3.54(3)O2···H1A ⁱⁱ 3.3418H14···C12 ⁱⁱⁱ 3.0895O2···H23A ⁱⁱⁱ 3.2088H14···H122A ⁱⁱⁱ 2.9242O2···H24C ⁱⁱ 2.8628H14···H12 ⁱⁱⁱ 3.0895O3···H1 ⁱⁱⁱ 3.5083H14···H22A ⁱⁱⁱ 2.9242O2···H24C ⁱⁱ 3.5868H15···H1 ⁱⁱⁱ 3.5543C7-O3-C8117.86 (16)C5-C4-H4A108.816C1-C2-C3118.84 (18)C5-C6-H6B108.870C1-C2-C3118.84 (18)C5-C6-H6B108.873C1-C2-C4117.42C6-G-G-H6B108.870C1-C2-C5113.74 (19) <t< td=""><td>H24B…H25A</td><td>3.5415</td><td>H25A…H18^v</td><td>2.6772</td></t<>	H24B…H25A	3.5415	H25A…H18 ^v	2.6772
$\begin{array}{llllllllllllllllllllllllllllllllllll$	H24B…H25B	2.4823	H25A…H24B ⁱⁱ	2.8715
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H24B…H25C	2.9505	H25A…H24C ⁱⁱ	2.9694
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H24C…H25B	3.5378	H25B…O1 ^{xi}	3.5309
H14H152.71 (4)H25BC16 ^{al} 3.2331F1H6A ^{al} 2.6922H25BC17 ^a 3.5667F1H6A ^{bl} 2.8599H25BH17 ^a 2.8858F1H20 ^a 3.0448H25BH18 ^a 3.1027O1H6A ⁱⁱ 3.0975H25BH18 ^a 3.2722O1H17 ⁱⁱ 2.8852H25CO1 ⁱⁱ 3.5911O1H23B ^{ai} 3.0772H25CC24 ^{ai} 3.4827O1H23B ^{ai} 3.0772H25CH23A ^{ai} 3.2102O1H23B ^{ai} 3.0534H25CH17 ^a 3.4576O1H23B ^{ai} 3.5911H25CH23A ^{ai} 3.2102O1H25B ^{ai} 3.5309H25CH23A ^{ai} 3.2102O1H25C ^{ai} 3.5911H25CH23A ^{ai} 3.2102O1H15 ⁱ 2.74 (3)H25CH24B ^{ai} 3.0227O2H4B ⁱⁱⁱ 3.0419H25CH24B ^{aii} 3.0227O2H4B ⁱⁱⁱ 3.0419H25C-H24C ^{aii} 3.1036O2H9B ⁱⁱⁱ 3.0258H14C17 ^{aii} 3.54 (3)O2H22B ^{aii} 2.6029H14H17 ⁱⁱ 3.0895O2H23A ^{aii} 3.2088H14H22A ^{aii} 2.9242O2H24C ^{ai} 2.8628H14H22B ^{aii} 2.6050O3H1 ^{iv} 3.5083H14H22B ^{aii} 2.6050O3H1 ^{iv} 3.548H15O1 ^{iv} 2.74 (3)O3H24C ^{ai} 3.5868H15H1 ^{iv} 3.5369O3H1 ^{iv} 3.5488H15O1 ^{iv} 2.74 (3)O3H20 ^{ai} 3.5868H15H1 ^{aiv} 3.5543C7-O3-C8117.86 (16)C5C4H4A108.870 <td>H24C…H25C</td> <td>3.5428</td> <td>H25B····C15^{xi}</td> <td>3.3106</td>	H24C…H25C	3.5428	H25B····C15 ^{xi}	3.3106
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H14…H15	2.71 (4)	H25B····C16 ^{xi}	3.2531
F1H6A ^{is} 3.2287 H25BC21 ^{si} 3.5623 F1H6B ⁱ 2.8599 H25BH17 ^v 2.8858 F1H20 ^c 3.0448 H25BH18 ^v 3.1027 O1H6A ⁱⁱⁱ 3.0975 H25BH23B ^{sii} 3.2722 O1H17 ⁱⁱ 2.8952 H25CC24 ⁱⁱ 3.4827 O1H23C ⁱⁱ 3.0772 H25CC24 ⁱⁱ 3.4827 O1H23B ⁱⁱ 3.0534 H25CH23A ^{sii} 3.2102 O1H25C ^{ix} 3.5911 H25CH23A ^{sii} 3.2102 O1H25C ^{ix} 3.5911 H25CH24C ⁱⁱⁱ 3.4810 O1H15 ⁱⁱ 2.74 (3) H25CH24C ⁱⁱⁱ 3.1036 O2H4B ⁱⁱⁱ 3.0419 H25CH24C ⁱⁱⁱ 3.1036 O2H4B ⁱⁱⁱ 3.0258 H14C17 ⁱⁱⁱ 3.54 (3) O2H22B ⁱⁱⁱⁱ 3.2088 H14H17 ⁱⁱⁱ 3.0895 O2H22B ⁱⁱⁱⁱ 3.6029 H14H17 ⁱⁱⁱ 3.0895 O2H22B ⁱⁱⁱⁱ 3.6053 H14H22B ⁱⁱⁱⁱ 2.9242 O2H22B ⁱⁱⁱⁱ 3.6053 H14H22B ⁱⁱⁱⁱ 2.6050 O3H12 ⁱⁱⁱ 3.5083 H14H22B ⁱⁱⁱⁱ	F1···H4A ⁱ	2.6922	H25B····C17 ^v	3.5667
F1H6B ⁱ 2.8599 H25BH17 [•] 2.8858 F1H6B ⁱ 2.8599 H25BH17 [•] 2.8858 F1H20 ^s 3.0448 H25B-·H13 st 3.1027 O1H6A ⁱⁱ 3.0975 H25B-·H23B st 3.2722 O1H17 ⁱⁱ 2.8952 H25C-··O1 st 3.5911 O1H23B ⁱⁱ 3.0772 H25C-··C24 ⁱⁱ 3.4827 O1H23C ⁱⁱ 3.0534 H25C-··H17 [•] 3.4576 O1H25D ^{is} 3.5309 H25C-··H23A ^{si} 3.2102 O1H25C ^{ix} 3.5911 H25C-··H23B ^{si} 3.4810 O1H15 ⁱⁱ 2.74 (3) H25C-··H24B ⁱⁱⁱ 3.0227 O2H4B ⁱⁱⁱ 3.0419 H25C-··H24B ⁱⁱⁱ 3.027 O2H4B ⁱⁱⁱ 3.0419 H25C-··H24C ⁱⁱ 3.1036 O2H4B ⁱⁱⁱ 3.0258 H14···C17 ⁱⁱⁱ 3.54 (3) O2H24B ⁱⁱⁱ 2.6029 H14···H17 ⁱⁱ 3.54 (3) O2H22B ⁱⁱⁱ 2.6029 H14···H22B ⁱⁱⁱ 2.6050 O3-··H1 ^{iv} 3.5083 H14···H22B ⁱⁱⁱ 2.6050 O3-··H1 ^{iv} 3.5083 H14···H22B ⁱⁱⁱ	F1···H6A ^{ix}	3.2287	H25B····C21 ^{xi}	3.5623
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F1···H6B ⁱ	2 8599	H25BH17 ^v	2.8858
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F1H20 ^x	3 0448	$H25B \cdots H18^{v}$	3 1027
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$01 \cdots H6A^{ii}$	3 0975	$H25B \cdots H23B^{xi}$	3 2722
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$01 \cdots H17^{ii}$	2 8952	$H_{25C} \cdots O_{1}^{x_i}$	3 5911
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$01 \cdots H23B^{ii}$	3 0772	$H25C \cdots C24^{ii}$	3 4827
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	01H23C ⁱⁱ	3 0534	H25CH17v	3 4576
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$01 \cdots H25B^{ix}$	3 5309	$H25C \cdots H23 A^{xi}$	3 2102
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$01 \cdots H25C^{ix}$	3 5911	H25CH23R ^{xi}	3 4810
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$01 - H15^{ii}$	2 74 (3)	H25C H24B ⁱⁱ	3.0227
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$02 \cdots H4B^{iii}$	3 0419	H25C H24D $H25C H24C^{ii}$	3 1036
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$02 \cdot H + B$	3 0258	H14C17 ⁱⁱ	3.1000
$O2 \dots H12B^{iii}$ $D.5.416$ $H14 \dots H17^{ii}$ $D.5.465$ $O2 \dots H22B^{iii}$ 2.6029 $H14 \dots H17^{ii}$ 3.0895 $O2 \dots H23A^{iii}$ 3.2088 $H14 \dots H22A^{iii}$ 2.9242 $O2 \dots H24C^{ii}$ 2.8628 $H14 \dots H22B^{iii}$ 2.6050 $O3 \dots H1^{iv}$ 3.5083 $H14 \dots H22B^{iii}$ 2.6050 $O3 \dots H1^{iv}$ 3.5083 $H14 \dots H22C^{vi}$ 3.5369 $O3 \dots H1^{iv}$ 3.5488 $H15 \dots O1^{iv}$ $2.74(3)$ $O3 \dots H20^{vi}$ 3.5868 $H15 \dots H1^{iv}$ 3.5543 C7O3C8 $117.86(16)$ C5C4H4A 108.816 C2C1C14 $112.04(15)$ $H4A$ C4H4B 108.809 C2C1C14 $110.00(17)$ C5C6H6A 108.873 C1C2C3 $118.84(18)$ C5C6H6B 108.870 C1C2C7 $122.35(18)$ C7C6H6B 108.879 C3C2C7 $118.81(18)$ C7C6H6B 108.878 O1C3C2 $121.1(2)$ $H6A$ C6H6B 107.714 O1C3C4 $121.5(3)$ $C8$ C9H9A 108.964 C2C3C4 $117.4(2)$ $C8$ C9H9B 108.960 C4C5C6 $108.50(17)$ $C10$ C9H9B 108.949	$02 \cdot H11 A^{ii}$	3 3418	H14····C22 ⁱⁱⁱ	3.0+(3)
$O2 \cdots H23A^{iii}$ 2.0025 $H14 \cdots H17$ 5.0055 $O2 \cdots H23A^{iii}$ 3.2088 $H14 \cdots H22A^{iii}$ 2.9242 $O2 \cdots H24C^{ii}$ 2.8628 $H14 \cdots H22B^{iii}$ 2.6050 $O3 \cdots H1^{iv}$ 3.5083 $H14 \cdots H22C^{vi}$ 3.5369 $O3 \cdots H1^{vv}$ 3.4484 $H15 \cdots O1^{iv}$ $2.74 (3)$ $O3 \cdots H20^{vi}$ 3.5868 $H15 \cdots H1^{iv}$ 3.5543 $C7 = O3 = C8$ $117.86 (16)$ $C5 = C4 = H4A$ 108.816 $C2 = C1 = C13$ $109.06 (17)$ $C5 = C4 = H4B$ 108.809 $C2 = C1 = C14$ $112.04 (15)$ $H4A = C4 = H4B$ 107.675 $C1 = C2 = C3$ $118.84 (18)$ $C5 = C6 = H6B$ 108.873 $C1 = C2 = C7$ $122.35 (18)$ $C7 = C6 = H6B$ 108.879 $C3 = C2 = C7$ $118.81 (18)$ $C7 = C6 = H6B$ 108.878 $O1 = C3 = C2$ $121.1 (2)$ $H6A = C6 = H6B$ 107.714 $O1 = C3 = C4$ $117.4 (2)$ $C8 = C9 = H9A$ 108.964 $C2 = C3 = C4$ $117.4 (19)$ $C10 = C9 = H9A$ 108.960 $C4 = C5 = C6$ $108.50 (17)$ $C10 = C9 = H9B$ 108.949	$02 \cdot H1111$	2 6029	H14H17 ⁱⁱ	3.0895
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	02H23A ⁱⁱⁱ	3 2088	$H14 \cdots H22 A^{iii}$	2 9242
$O2 \cdot H2+C$ 2.0020 $H1+H22D$ 2.0030 $O3 \cdots H1^{iv}$ 3.5083 $H14 \cdots H22C^{vi}$ 3.5369 $O3 \cdots H18^{v}$ 3.4484 $H15 \cdots O1^{iv}$ $2.74 (3)$ $O3 \cdots H20^{vi}$ 3.5868 $H15 \cdots H1^{iv}$ 3.5543 $C7 - O3 - C8$ $117.86 (16)$ $C5 - C4 - H4A$ 108.816 $C2 - C1 - C13$ $109.06 (17)$ $C5 - C4 - H4B$ 108.809 $C2 - C1 - C14$ $112.04 (15)$ $H4A - C4 - H4B$ 107.675 $C13 - C1 - C14$ $110.00 (17)$ $C5 - C6 - H6A$ 108.870 $C1 - C2 - C3$ $118.84 (18)$ $C5 - C6 - H6B$ 108.879 $C3 - C2 - C7$ $122.35 (18)$ $C7 - C6 - H6B$ 108.878 $O1 - C3 - C2$ $121.1 (2)$ $H6A - C6 - H6B$ 107.714 $O1 - C3 - C4$ $121.5 (3)$ $C8 - C9 - H9A$ 108.964 $C2 - C3 - C4$ $117.4 (2)$ $C8 - C9 - H9B$ 108.960 $C4 - C5 - C6$ $108.50 (17)$ $C10 - C9 - H9B$ 108.949	$02 \cdots H24C^{ii}$	2 8628	H14H22R	2.5212
$O3 \cdots H1^8v$ 3.4484 $H15 \cdots O1^{iv}$ $2.74 (3)$ $O3 \cdots H20^{xi}$ 3.5868 $H15 \cdots H1^{iv}$ 3.5543 $C7 = O3 = C8$ $117.86 (16)$ $C5 = C4 = H4A$ 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 $C1 = C2 = C7$ $122.35 (18)$ $C7 = C6 = H6B$ 108.879 $O1 = C3 = C2$ $121.1 (2)$ $H6A = C6 = H6B$ 108.878 $O1 = C3 = C4$ $121.5 (3)$ $C8 = C9 = H9A$ 108.964 $C2 = C3 = C4$ $117.4 (2)$ $C8 = C9 = H9B$ 108.967 $C3 = C4 = C5$ $113.74 (19)$ $C10 = C9 = H9B$ 108.949	03···H1 ^{iv}	3 5083	$H14\cdots H22C^{vi}$	3 5369
$O3 - H20^{xi}$ 3.440^{xi} $H15 - O1^{xi}$ $2.74(5)^{xi}$ $O3 - H20^{xi}$ 3.5868 $H15 - H1^{iv}$ 3.5543 $C7 - O3 - C8$ $117.86(16)$ $C5 - C4 - H4A$ 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 $C1 - C2 - C7$ $122.35(18)$ $C7 - C6 - H6B$ 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 $C3 - C4 - C5$ $113.74(19)$ $C10 - C9 - H9B$ 108.949	03H18 ^v	3 4484	H1501 ^{iv}	2.5507
C7-O3-C8117.86 (16)C5-C4-H4A108.816C2-C1-C13109.06 (17)C5-C4-H4B108.809C2-C1-C14112.04 (15)H4A-C4-H4B107.675C13-C1-C14110.00 (17)C5-C6-H6A108.873C1-C2-C3118.84 (18)C5-C6-H6B108.870C1-C2-C7122.35 (18)C7-C6-H6B108.878C1-C3-C2118.81 (18)C7-C6-H6B108.878O1-C3-C2121.1 (2)H6A-C6-H6B107.714O1-C3-C4121.5 (3)C8-C9-H9A108.964C2-C3-C4117.4 (2)C8-C9-H9B108.967C3-C4-C5113.74 (19)C10-C9-H9B108.949	$03 \cdots H20^{xi}$	3 5868	H15H1iv	2.74 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	05 1120	5.5000		5.5545
C2-C1-C13109.06 (17)C5-C4-H4B108.809C2-C1-C14112.04 (15)H4A-C4-H4B107.675C13-C1-C14110.00 (17)C5-C6-H6A108.873C1-C2-C3118.84 (18)C5-C6-H6B108.870C1-C2-C7122.35 (18)C7-C6-H6B108.879C3-C2-C7118.81 (18)C7-C6-H6B108.878O1-C3-C2121.1 (2)H6A-C6-H6B107.714O1-C3-C4121.5 (3)C8-C9-H9A108.964C2-C3-C4117.4 (2)C8-C9-H9B108.967C3-C4-C5113.74 (19)C10-C9-H9B108.949	C7—O3—C8	117.86 (16)	C5—C4—H4A	108.816
C2-C1-C14112.04 (15)H4A-C4-H4B107.675C13-C1-C14110.00 (17)C5-C6-H6A108.873C1-C2-C3118.84 (18)C5-C6-H6B108.870C1-C2-C7122.35 (18)C7-C6-H6B108.879C3-C2-C7118.81 (18)C7-C6-H6B108.878O1-C3-C2121.1 (2)H6A-C6-H6B107.714O1-C3-C4121.5 (3)C8-C9-H9A108.964C2-C3-C4117.4 (2)C8-C9-H9B108.967C3-C4-C5113.74 (19)C10-C9-H9B108.949	C2—C1—C13	109.06 (17)	C5—C4—H4B	108.809
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—C1—C14	112.04 (15)	H4A—C4—H4B	107.675
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—H9B 108.960 C4—C5—C6 108.50 (17) C10—C9—H9B 108.949	C13—C1—C14	110.00 (17)	С5—С6—Н6А	108.873
C1C2C7 122.35 (18) C7C6H6A 108.879 C3C2C7 118.81 (18) C7C6H6B 108.878 O1C3C2 121.1 (2) H6AC6H6B 107.714 O1C3C4 121.5 (3) C8C9H9A 108.964 C2C3C4 117.4 (2) C8C9H9B 108.967 C3C4C5 113.74 (19) C10C9H9B 108.960 C4C5C6 108.50 (17) C10C9H9B 108.949	C1—C2—C3	118.84 (18)	С5—С6—Н6В	108.870
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	C1—C2—C7	122.35 (18)	С7—С6—Н6А	108.879
O1—C3—C2121.1 (2)H6A—C6—H6B107.714O1—C3—C4121.5 (3)C8—C9—H9A108.964C2—C3—C4117.4 (2)C8—C9—H9B108.967C3—C4—C5113.74 (19)C10—C9—H9A108.960C4—C5—C6108.50 (17)C10—C9—H9B108.949	C3—C2—C7	118.81 (18)	С7—С6—Н6В	108.878
O1C3C4121.5 (3)C8C9H9A108.964C2C3C4117.4 (2)C8C9H9B108.967C3C4C5113.74 (19)C10C9H9A108.960C4C5C6108.50 (17)C10C9H9B108.949	O1—C3—C2	121.1 (2)	H6A—C6—H6B	107.714
C2-C3-C4117.4 (2)C8-C9-H9B108.967C3-C4-C5113.74 (19)C10-C9-H9A108.960C4-C5-C6108.50 (17)C10-C9-H9B108.949	O1—C3—C4	121.5 (3)	С8—С9—Н9А	108.964
C3—C4—C5113.74 (19)C10—C9—H9A108.960C4—C5—C6108.50 (17)C10—C9—H9B108.949	C2—C3—C4	117.4 (2)	С8—С9—Н9В	108.967
C4—C5—C6 108.50 (17) C10—C9—H9B 108.949	C3—C4—C5	113.74 (19)	С10—С9—Н9А	108.960
	C4—C5—C6	108.50 (17)	С10—С9—Н9В	108.949
С4—С5—С22 111.7 (2) Н9А—С9—Н9В 107.764	C4—C5—C22	111.7 (2)	Н9А—С9—Н9В	107.764
C4—C5—C23 108.13 (18) C10—C11—H11A 108.599	C4—C5—C23	108.13 (18)	C10-C11-H11A	108.599

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
C_{24} C_{10} C_{25}	109.18 (17)	C5—C22—H22A	109.474
C10-C11-C12	114.68 (17)	C5—C22—H22B	109.466
02-C12-C11	121.55 (19)	C5—C22—H22C	109.466
0^{2} - C12 - C13	120.7(2)	H22A-C22-H22B	109 474
$C_{11} - C_{12} - C_{13}$	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		
C7—O3—C8—C9	-172 44 (13)	03	159 36 (13)
C7-03-C8-C13	78(3)	03 - C8 - C13 - C1	4 2 (3)
$C_{8} = O_{3} = C_{7} = C_{2}^{2}$	-70(3)	03 - C8 - C13 - C12	-17908(14)
$C_{3} = C_{1} = C_{2}$	172 (8)	C9 - C8 - C13 - C12	-17550(14)
C_{2} C_{1} C_{13} C_{8}	-150(3)	C_{9} C_{8} C_{13} C_{12}	12(3)
$C_2 - C_1 - C_{13} - C_{12}$	168 36 (14)	C_{13} C_{8} C_{9} C_{10}	-200(2)
C2-C1-C13-C12	100.30 (14)	013-00-09-010	-20.9 (3)

C13—C1—C2—C3 C13—C1—C2—C7	-164.10 (14) 15 7 (3)	C8—C9—C10—C11 C8—C9—C10—C24	44.1 (2) 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, °)

D—H···A	<i>D</i> —Н	H···A	D····A	<i>D</i> —H··· <i>A</i>
C22—H22 B ···O2 ^{vii}	0.96	2.60	3.533 (4)	163

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