Synthesis, characterization, crystal structure and Hirshfeld surface analysis of a hexahydroquinoline derivative: tert-butyl 4-((1,1'-biphenyl)-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate

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The title compound, C_{29}H_{33}NO_{3}, crystallizes with three molecules (A, B and C) in the asymmetric unit. They differ in the twist of the phenyl and benzene rings of the 1,1'-biphenyl ring with respect to the plane of the 1,4-dihydropyridine ring. In all three molecules, the 1,4-dihydropyridine ring adopts a distorted boat conformation. The cyclohexene ring has an envelope conformation in molecules A and B, while it exhibits a distorted half-chair conformation for both the major and minor components in the disordered molecule C. In the crystal, molecules are linked by C—H···O and N—H···O hydrogen bonds, forming layers parallel to (100) defining R_{1}(6) and C(7) graph-set motifs. Additional C—H···π interactions consolidate the layered structure. Between the layers, van der Waals interactions stabilize the packing, as revealed by Hirshfeld surface analysis. The greatest contributions to the crystal packing are from H···H (69.6% in A, 69.9% in B, 70.1% in C), C···H/H···C (20.3% in A, 20.6% in B, 20.3% in C) and O···H/H···O (8.6% in A, 8.6% in B, 8.4% in C) interactions.

1. Chemical context

Chronic diseases are among the most common causes of death in the world, accompanied by difficulties and costs in treatment and health care. Therefore, preventing or treating chronic diseases is of paramount importance (Raghupathi & Raghupathi, 2018). Recent advances have shown that many diseases such as cancer, atherosclerosis or neurodegenerative diseases are triggered by inflammation (Furman et al., 2019). Based on these findings, regulating inflammatory mediators and pathways has been suggested as a treatment strategy (Kany et al., 2019).

Inflammatory stimuli that cause chronic inflammation initiate the production of inflammatory mediators such as interleukin-1β (IL-1β), interleukin-6 (IL-6) and tumor necrosis factor-α (TNF-α) as a result of the activation of signaling pathways. Receptors activated by inflammatory mediators induce chronic inflammation by various signaling pathways (nuclear factor κ-B (NF-KB), Janus kinase (JAK), signal transducer and activator of transcription (STAT),...
Inhibiting these pathways may be a promising approach for the treatment of chronic diseases associated with inflammation (Chen et al., 2018).

Nifedipine, the first drug with a 1,4-dihydropyridine (1,4-DHP) ring, was introduced as a therapeutic agent as a result of intensive studies. The success of nifedipine as an antihypertensive drug has led to further studies and the discovery of other 1,4-DHP derivatives (De Luca et al., 2019). Numerous compounds were obtained through modifications with respect to the 1,4-DHP ring. These studies also uncovered the idea of obtaining hexahydroquinoline derivatives by condensation of the 1,4-DHP scaffold with the cyclohexane ring system (Bladen et al., 2014). In recent years, it has been found that 1,4-DHP and quinoline analogs have the potential to inhibit inflammation mediators and pathways, along with various other pharmacological activities (Costa et al., 2010; Längle et al., 2015; Kim et al., 2018; Çetin et al., 2022).

In the current study, tert-butyl 4-{[1,1'-biphenyl]-4-yl}-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate was obtained by condensation of the 1,4-DHP ring with a substituted cyclohexane ring using a modified Hantzsch method. The molecular structure of the compound was confirmed by spectroscopic methods such as IR, $^1$H NMR, $^{13}$C NMR, and its composition by elemental analysis. In addition, single-crystal X-ray analysis was performed to elucidate the crystal structure of the compound. Independent of the current study, biological activity studies of the title compound are ongoing.

### 2. Structural commentary

The asymmetric unit of the title compound (Fig. 1) contains three independent molecules (denoted with suffixes $A$, $B$ and $C$).
C). They mainly differ in the twist of the phenyl (C24–C29) and benzene (C18–C23) rings of the 1,1′-biphenyl ring with respect to the plane of the 1,4-dihydropyridine ring (N1/C1–C4/C9). The corresponding dihedral angles amount to 89.26 (16) and 75.83 (19)° in molecule A, 88.34 (17) and 71.7 (2)° in molecule B, and 89.38 (17) and 83.6 (3)° in molecule C. The phenyl and benzene rings of the 1,1′-biphenyl ring make dihedral angles of 39.05 (19)° in A, 46.9 (2)° in B, and 33.5 (2)° in C. Fig. 2 shows an overlay plot of molecules A, B, and C, with an r.m.s. deviation of 0.725 Å. Except for the atoms of the minor part of the disordered molecule C and the phenyl ring of the biphenyl group, the other atoms of molecule C and all atoms of molecules A and B are quite compatible and coincide with each other.

In all three molecules, the 1,4-dihydropyridine ring adopts a distorted boat conformation with puckering parameters (Cremer & Pople, 1975) \( Q_T = 0.269 (4) \) Å, \( \theta = 104.5 (9) \)° and \( \varphi = 357.4 (9) \)° in A, \( Q_T = 0.257 (4) \) Å, \( \theta = 73.1 (9) \)° and \( \varphi = 176.0 (9) \)° in B, and \( Q_T = 0.303 (4) \) Å, \( \theta = 106.9 (8) \)° and \( \varphi = 356.2 (8) \)° in C. The cyclohexene ring (C4–C9) has an envelope conformation in molecules A and B [the puckering parameters are \( Q_T = 0.430 (4) \) Å, \( \theta = 49.3 (5) \)° and \( \varphi = 182.3 (7) \)° in A, and \( Q_T = 0.439 (4) \) Å, \( \theta = 58.8 (5) \)° and \( \varphi = 179.9 (6) \)° in B], while the major and minor components of the disordered cyclohexene rings in C exhibit a distorted half-chair conformation, with puckering parameters of \( Q_T = 0.451 (9) \) Å, \( \theta = 44.7 (12) \)° and \( \varphi = 161 (2) \)° for the major component, and of \( Q_T = 0.44 (2) \) Å, \( \theta = 50 (3) \)° and \( \varphi = 206 (5) \)° for the minor component.

Bond lengths and angles in the three molecules of the title compound are comparable with those of closely related structures detailed in section 5 (Database survey).

3. Supramolecular features

In the crystal, molecules are linked by C—H···O and N—H···O hydrogen bonds (Table 1, Fig. 3), forming layers parallel to (100), defining \( R_2(6) \) and \( C(7) \) graph-set motifs (Bernstein et al., 1995). Additional C—H···π interactions consolidate the layered arrangement (Table 1; Fig. 4). Between the layers, van der Waals interactions stabilize the packing, as revealed by Hirshfeld surface analysis.

4. Hirshfeld surface analysis

Crystal Explorer 17.5 (Spackman et al., 2021) was used to construct Hirshfeld surfaces for the three independent molecules; the disorder of molecule C was included in the calculations. The \( d_{norm} \) mappings for molecule A were performed in the range \(-0.5982 \) to \(+2.4710 \) a.u., for molecule B in the range

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**Table 1**

Hydrogen-bond geometry (Å, °).

| D—H···A   | D—H | H···A | D···A | D—H···A |
|-----------|-----|------|-------|---------|
| N1−H1A···O1B | 0.92 (5) | 1.94 (5) | 2.843 (4) | 165 (5) |
| N1B−H1NB···O1C | 0.95 (4) | 1.88 (4) | 2.811 (4) | 168 (3) |
| N1A−H1NA···O1A | 0.93 (5) | 1.92 (5) | 2.842 (4) | 174 (4) |
| C10A−H10B···O1A | 0.98 | 2.60 | 3.443 (5) | 145 |
| C10B−H10F···O1C | 0.98 | 2.47 | 3.302 (5) | 143 |
| C13A−H13A···O2A | 0.98 | 2.45 | 2.978 (7) | 113 |
| C13B−H13D···O2B | 0.98 | 2.47 | 3.023 (6) | 115 |
| C15A−H15A···O2A | 0.98 | 2.41 | 2.999 (7) | 118 |
| C15B−H15D···O2B | 0.98 | 2.41 | 2.965 (6) | 116 |
| C15C−H15G···O2C | 0.98 | 2.49 | 3.022 (5) | 114 |
| C23A−H23A···O2A | 0.95 | 2.57 | 3.403 (4) | 147 |
| C23B−H23B···O2C | 0.95 | 2.55 | 3.389 (5) | 147 |
| C23C−H23C···O2B | 0.95 | 2.60 | 3.407 (4) | 144 |
| C15A−H15B···C13A | 0.98 | 2.82 | 3.771 (6) | 165 |
| C27A−H27A···C4A | 0.95 | 2.75 | 3.578 (4) | 146 |
| C27B−H27B···C8 | 0.95 | 2.63 | 3.493 (5) | 150 |
| C27C−H27C···C41A | 0.95 | 2.84 | 3.632 (7) | 142 |

Symmetry codes: (i) \( x, y, z - 1 \); (ii) \(-x + 1, y, z + 1/2\); (iii) \(-x + 1, y, z - 1/2\).
Table 2
Summary of short interatomic contacts (Å) in the title compound.

| Contact         | Distance | Symmetry operation |
|-----------------|----------|--------------------|
| O1C···H1NB      | 1.88     | x, y, z            |
| H1NC···O1B      | 1.94     | x, y, -1 + z       |
| H10f···H14B     | 2.40     | 1 - x, 1 - y, -1/2 + z |
| C8C···H16K      | 3.07     | 1 - x, -y, -1/2 + z |
| H10G···H13H     | 2.43     | 1 - x, 1 - y, -1/2 + z |
| C19C···H27A     | 2.86     | 1/2 - x, y, -1/2 + z |
| H26C···C20B     | 2.90     | 1/2 - x, y, -1/2 + z |
| H17K···H10E     | 2.07     | 1 - x, -y, -1/2 + z |
| H16G···H17A     | 2.52     | 1/2 - x, -1 + y, -1/2 + z |
| H20C···H28C     | 2.56     | 1/2 - x, y, -1/2 + z |
| O1A···H1NA      | 1.92     | 1/2 - x, y, -1/2 + z |
| H7A···H15E      | 2.49     | x, 1 + y, z        |
| H10B···H17D     | 2.51     | 1 - x, 1 - y, 1/2 + z |
| H16A···H17F     | 2.47     | -1/2 + x, 1 - y, z |
| C19A···H27B     | 2.89     | x, y, z            |
| H16B···C10B     | 2.97     | 1/2 - x, y, -1/2 + z |
| H28A···H20B     | 2.42     | 1/2 - x, y, -1/2 + z |

Table 3
Percentage contributions of interatomic contacts to the Hirshfeld surfaces for the molecules A, B and C of the title compound.

| Contact         | % for A | % for B | % for C |
|-----------------|---------|---------|---------|
| H···H            | 69.6    | 69.9    | 70.1    |
| C···H/···C       | 20.3    | 20.6    | 20.3    |
| O···H/···O       | 8.6     | 8.6     | 8.4     |
| N···H/···N       | 1.1     | 0.8     | 0.9     |
| C···C            | 0.5     | 0.1     | 0.4     |

Figure 5
(a) View of the three-dimensional Hirshfeld surface for molecule A; (b) view of the three-dimensional Hirshfeld surface for molecule B; (c) view of the three-dimensional Hirshfeld surface for molecule C. Some intermolecular N···H and C···H···O interactions are shown as dashed lines.

Figure 6
The two-dimensional fingerprint plots for molecules A, B and C showing (a) all interactions, and delineated into (b) H···H, (c) C···H····C and (d) O···H/···O interactions. The di and dj values are the closest internal and external distances (Å) from given points on the Hirshfeld surface.

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Contact distances and symmetry operations are shown as dashed lines. The contact distances range from 0.5 to 2.5 Å, and the symmetry operations describe the locations of H···H and C···H···O interactions. The Hirshfeld surfaces (Fig. 5) reveal the locations of these interactions, with bright-red spots indicating the closest distances. Fingerprint plots (Fig. 6) show the contributions of each interaction type, with H···H interactions making the largest contributions. Some intermolecular N···H and C···H···O interactions are also significant. The two-dimensional fingerprint plots (Fig. 6) disclose the frequencies of these interactions, highlighting the importance of H···H and C···H···O interactions in the crystal structure.
5. Database survey
A search of the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; Groom et al., 2016) for similar structures with the 1,4,5,6,7,8-hexahydroquinoline unit revealed seven closely related entries: ethyl 4-(4-bromophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate [CSD refcode LOQCAX (I); Steiger et al., 2014], ethyl 4-(3-hydroxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate [PUGCIE (II); Moohkia et al., 2009], (RR,SS)-methyl 4-(2,4-chlorophenyl)-2,7-dimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (RS,SR)-methyl 4-(2,4-chlorophenyl)-2,7-dimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate [UCOLOO (III); Linden et al., 2006], ethyl 2,7,7-trimethyl-4-(1-methyl-1H-indol-3-yl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate [NEQMON (IV); Oztürel Yildirim et al., 2013], (+/−)-methyl 4-(2,3-difluorophenyl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate [DAYJET (V); Linden et al., 2005], benzyl 4-(3-chloro-2-fluorophenyl)-2-methyl-5-oxo-4,5,6,7-tetrahydro-1H-cyclopenta[b]pyridine-3-carboxylate [IMEJOA (VI); Linden et al., 2011], and ethyl 4-(5-bromo-1H-indol-3-yl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate [PECPUK (VII); Gündüz et al., 2012].

In (I), hydrogen bonds are formed between the N−H group of one molecule and the carbonyl O atom in the cyclohexalone ring of an adjacent molecule. These hydrogen bonds link the molecules into extended chains running along [001]. In the crystal of (II), molecules are linked by N—H⋅⋅⋅O and O—H⋅⋅⋅O hydrogen bonds into layers parallel to (011). The network includes R$_2^2$(30) and R$_2^2$(34) graph-set motifs. In (III), an intermolecular N−H⋅⋅⋅O hydrogen bond between the amine group and the carbonyl O atom of the cyclohexalone ring of a neighboring molecule links the molecules into extended chains parallel to [010]. These interactions can be described by graph-set motif C(6). In the crystal of (IV), N−H⋅⋅⋅O hydrogen bonds connect the molecules into C(6) chains parallel to [010], and pairs of weak C−H⋅⋅⋅O hydrogen bonds link inversion-related chains into a ladder motif through R$_3^2$(18) rings. A weak intramolecular C−H⋅⋅⋅O hydrogen bond is also observed. In (V), the crystal structure exhibits an intermolecular N−H⋅⋅⋅O hydrogen-bonding interaction involving the carbonyl O atom of the oxocyclohexene ring, whereby the molecules are linked into C(6) chains parallel to [100]. In (VI), the frequently observed intermolecular N−H⋅⋅⋅O hydrogen bond between the amine group and the carbonyl O atom of the oxocyclopentene ring of a neighboring molecule links the molecules into extended C(6) chains parallel to [010]; there are no other significant intermolecular interactions. In the crystal of (VII), molecules are linked by pairs of N−H⋅⋅O hydrogen bonds, forming dimers with R$_2^2$(6) ring motifs. These dimers are connected by N−H⋅⋅⋅O hydrogen bonds, generating chains along [110]. A C−H⋅⋅⋅O contact occurs between the independent molecules.

6. Synthesis and crystallization
The title compound was synthesized via a Hantzsch reaction. 4,4-Dimethylcyclohexene-1,3-dione (1 mmol), [1,1′-biphenyl]-4-carboxaldehyde (1 mmol), tert-butyl acetoacetate (1 mmol), and ammonium acetate (5 mmol) were refluxed for 8 h in absolute methanol (10 ml). The reaction mixture was monitored by TLC, and after completion of the reaction was cooled to room temperature. The obtained precipitate was filtered and recrystallized from ethanol for further purification. The synthetic route is shown in Fig. 7.

Yellowish solid, m.p. 520-522 K; yield: 41%. IR (v, cm$^{-1}$) 3284 (N−H stretching), 3067 (C−H stretching, aromatic), 2966 (C−H stretching, aliphatic) 1671 (C=O stretching, ester), 1597 (C=O stretching, ketone). $^1$H NMR (DMSO-d$_6$) δ: 0.88 (3H; 6-CH$_3$), 0.97 (3H; 6-CH$_3$), 1.32 [9H, s, C(CH$_3$)$_3$], 1.70–1.71 (2H; m; quinoline H7), 2.23 (3H; s; 2-CH$_3$), 2.47–2.50 (2H; m; quinoline H8), 4.82 (1H; s; quinoline H4), 7.19–7.21 (2H, m, Ar-H), 7.27–7.31 (H, m, Ar-H), 7.38–7.48 (4H, m, Ar-H), 7.57–7.59 (2H, m, Ar-H), 8.98 (1H, s; NH). $^{13}$C NMR (DMSO-d$_6$) δ: 18.2, 22.9, 24.1, 25.1, 27.9, 34.1, 36.0, 40.0, 78.7, 104.6, 108.8, 126.0, 126.3, 127.0, 127.9, 128.7, 137.3, 140.1, 143.8, 147.1, 149.8, 166.4, 199.3. Analysis calculated for C$_{26}$H$_{33}$NO$_3$: C 78.52, H 7.5, N 3.16. Found: C 78.30, H 7.602, N 3.19.

7. Refinement details
Crystal data, data collection and structure refinement details are summarized in Table 4. All C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms, with C−H = 0.95 Å for aryl-H atoms, C−H = 0.99 Å for methylene groups, C−H = 1.00 Å for methine groups and C−H = 0.98 Å for methyl groups, with $U_{iso}(H)$ = 1.5$U_{eq}(C)$ for methyl groups and $U_{iso}(H)$ = 1.2$U_{eq}(C)$ for other hydrogen atoms. The H atoms of the NH groups were found in a difference-Fourier map and refined freely (see Table 1).

In molecule C, except the fused carbon atoms (C4C and C9C) and the carbonyl oxygen atom (O1C) of the 6,6-dimethylocyclohex-2-en-1-one group (C4C–C5C/C5F–C6C/C6F–C7C/C7F–C8C/C8F–C9C–O1C–C16C/C16F–C17C/C17F), the other C atoms are disordered over two sets of sites with a refined occupancy ratio of 0.716 (4):0.284 (4). For the disordered components, the EADP instruction was used in the final cycles of the refinement.

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Table 4
Experimental details.

| Crystal data | Chemical formula | C_{29}H_{33}NO_3 |
|--------------|------------------|-----------------|
| M_e          |                  | 443.56          |
| Crystal system, space group | Orthorhombic, Pca_2_1 |
| Temperature (K) |                  | 100             |
| a, b, c (Å) |                   | 32.2274 (14), 19.0904 (7), 12.0370 (3) |
| V (Å³)  |                   | 7634.7 (5)      |
| Z          |                   | 12              |
| Radiation type | Mo K              |
| μ (mm⁻¹)  |                   | 0.07            |
| Crystal size (mm) |               | 0.29 × 0.17 × 0.04 |

Data collection

| Diffractometer | SuperNova, Dual, Cu at zero, Atlas CrysAlis PRO (Rigaku OD, 2015) |
| Rint         | 0.091                                                              |
| R(max)       | 0.815                                                              |

| Rint | 0.091 |
| R(max) | 0.815 |

Refinement

| R[<i>F</i>² > 2σ(<i>F</i>²)], wR(<i>F</i>²), S | 0.077, 0.212, 1.02 |
| No. of reflections | 26062 |
| No. of parameters | 943 |
| No. of restraints | 13 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| Δρ(max), Δρ(min) (e Å⁻³) | 0.58, -0.37 |

Computer programs: CrysAlis PRO (Rigaku OD, 2015), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), ORTEP-3 for Windows (Farrugia, 2012), and PLATON (Spek, 2020).

Conceptualization, RS and SOY; methodology, RS and GC; investigation, RS and SOY; writing (original draft), GC and MA writing (review and editing of the manuscript), RS and SOY; crystal data production and validation, RJB and SOY; visualization, MA; funding acquisition, RJB; resources, AB, RJB and RS.

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Synthesis, characterization, crystal structure and Hirshfeld surface analysis of a hexahydroquinoline derivative: tert-butyl 4-([1,1′-biphenyl]-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate

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Computing details
Data collection: CrysAlis PRO (Rigaku OD, 2015); cell refinement: CrysAlis PRO (Rigaku OD, 2015); data reduction: CrysAlis PRO (Rigaku OD, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: SHELXL (Sheldrick, 2015b); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication: PLATON (Spek, 2020).

tert-Butyl 4-([1,1′-biphenyl]-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate

Crystal data
C_{29}H_{33}NO_{3}  
Mr = 443.56  
Orthorhombic, Pca_{2}1  
a = 33.2247 (14) Å  
b = 19.0904 (7) Å  
c = 12.0370 (3) Å  
V = 7634.7 (5) Å^3  
Z = 12  
F(000) = 2856

Data collection
SuperNova, Dual, Cu at zero, Atlas diffractometer  
Radiation source: micro-focus sealed X-ray tube  
Detector resolution: 10.6501 pixels mm^{-1}  
69430 measured reflections  
26062 independent reflections  
13388 reflections with I > 2\sigma(I)

Refinement
Refinement on F^2  
Least-squares matrix: full  
R[F^2 > 2\sigma(F^2)] = 0.077  
wR(F^2) = 0.212  
S = 1.02  
943 parameters  
13 restraints  
Hydrogen site location: mixed  
H atoms treated by a mixture of independent and constrained refinement

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**supporting information**

\[ w = \frac{1}{\sigma^2(F_o^2) + (0.0858P)^2 + 0.3289P} \]
where \[ P = (F_o^2 + 2F_c^2)/3 \]
\[ \Delta \rho_{\text{max}} = 0.58 \text{ e Å}^{-3} \]
\[ \Delta \rho_{\text{min}} = -0.37 \text{ e Å}^{-3} \]
\[ (\Delta / \sigma)_{\text{max}} < 0.001 \]

**Special details**

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

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

|     | x     | y     | z     | \( U_{iso} ^* / U_{eq} \) | Occ. (<1) |
|-----|-------|-------|-------|---------------------------|-----------|
| O1C | 0.46360 (9) | 0.08706 (13) | 0.3497 (2) | 0.0319 (6) |          |
| O2C | 0.45841 (11) | 0.33966 (14) | 0.4075 (2) | 0.0401 (8) |          |
| O3C | 0.48150 (10) | 0.41061 (13) | 0.2723 (2) | 0.0333 (7) |          |
| N1C | 0.48126 (9) | 0.24320 (15) | 0.0522 (2) | 0.0210 (6) |          |
| H1NC | 0.4898 (17) | 0.253 (3) | −0.019 (4) | 0.054 (15)* |          |
| C1C | 0.47707 (11) | 0.30241 (18) | 0.1187 (3) | 0.0217 (7) |          |
| C2C | 0.46516 (11) | 0.29472 (18) | 0.2253 (3) | 0.0215 (7) |          |
| C3C | 0.44911 (11) | 0.22483 (17) | 0.2661 (3) | 0.0195 (6) |          |
| H3CA | 0.457116 | 0.219390 | 0.345766 | 0.023* |          |
| C4C | 0.46876 (12) | 0.16588 (18) | 0.2003 (3) | 0.0223 (7) |          |
| C9C | 0.48166 (11) | 0.17716 (18) | 0.0953 (3) | 0.0216 (7) |          |
| C10C | 0.48761 (13) | 0.36843 (19) | 0.0585 (3) | 0.0280 (8) |          |
| H10G | 0.469779 | 0.406270 | 0.083077 | 0.042* |          |
| H10H | 0.484358 | 0.361273 | −0.021631 | 0.042* |          |
| H10I | 0.515606 | 0.381025 | 0.074573 | 0.042* |          |
| C11C | 0.46732 (13) | 0.34996 (18) | 0.3106 (3) | 0.0252 (8) |          |
| C12C | 0.48964 (15) | 0.4703 (2) | 0.3458 (3) | 0.0363 (10) |          |
| C13C | 0.52017 (17) | 0.4500 (3) | 0.4339 (4) | 0.0531 (14) |          |
| H13G | 0.506416 | 0.426122 | 0.495179 | 0.080* |          |
| H13H | 0.533542 | 0.492149 | 0.461951 | 0.080* |          |
| H13I | 0.540253 | 0.418457 | 0.401344 | 0.080* |          |
| C14C | 0.5076 (2) | 0.5231 (2) | 0.2654 (4) | 0.0633 (17) |          |
| H14G | 0.489180 | 0.529980 | 0.202794 | 0.095* |          |
| H14H | 0.533472 | 0.505606 | 0.237940 | 0.095* |          |
| H14I | 0.511733 | 0.567845 | 0.303760 | 0.095* |          |
| C15C | 0.45081 (16) | 0.4972 (2) | 0.3945 (4) | 0.0455 (12) |          |
| H15G | 0.440597 | 0.463492 | 0.449029 | 0.068* |          |
| H15H | 0.430940 | 0.503272 | 0.335077 | 0.068* |          |
| H15I | 0.455634 | 0.542314 | 0.430975 | 0.068* |          |
| C5C | 0.4736 (4) | 0.0987 (5) | 0.2485 (11) | 0.0182 (16) | 0.716 (4) |
| C6C | 0.4829 (2) | 0.0353 (4) | 0.1732 (5) | 0.0231 (13) | 0.716 (4) |
| C7C | 0.51262 (18) | 0.0589 (3) | 0.0831 (4) | 0.0254 (10) | 0.716 (4) |
| H7CA | 0.538459 | 0.071720 | 0.118645 | 0.030* | 0.716 (4) |
| H7CB | 0.517837 | 0.019137 | 0.032286 | 0.030* | 0.716 (4) |
| C8C | 0.497 (7) | 0.1206 (6) | 0.0158 (11) | 0.0219 (16) | 0.716 (4) |
| H8CA | 0.475884 | 0.105316 | −0.034922 | 0.026* | 0.716 (4) |
| Atom   | x      | y      | z      | Ueq  |
|--------|--------|--------|--------|------|
| C     | 0.44347 (19) | 0.0096 (3) | 0.1220 (5) | 0.0.026* |
| H     | 0.519848 | 0.139966 | −0.029617 | 0.716 (4) |
| C     | 0.430524 | 0.048234 | 0.081918 | 0.052* |
| H     | 0.449072 | 0.028783 | 0.070302 | 0.052* |
| C     | 0.5016 (2) | −0.0234 (3) | 0.2432 (5) | 0.0392 (14) |
| H     | 0.483035 | −0.036371 | 0.0679 (10) | 0.054 (10) |
| H     | 0.425520 | −0.006979 | 0.181001 | 0.052* |
| C     | 0.44347 (19) | 0.0096 (3) | 0.1220 (5) | 0.0.026* |
| H     | 0.519848 | 0.139966 | −0.029617 | 0.716 (4) |
| C     | 0.430524 | 0.048234 | 0.081918 | 0.052* |
| H     | 0.449072 | 0.028783 | 0.070302 | 0.052* |
| C     | 0.5016 (2) | −0.0234 (3) | 0.2432 (5) | 0.0392 (14) |
| H     | 0.483035 | −0.036371 | 0.0679 (10) | 0.054 (10) |
| H     | 0.425520 | −0.006979 | 0.181001 | 0.052* |
| C     | 0.44347 (19) | 0.0096 (3) | 0.1220 (5) | 0.0.026* |
| H     | 0.519848 | 0.139966 | −0.029617 | 0.716 (4) |
| C     | 0.430524 | 0.048234 | 0.081918 | 0.052* |
| H     | 0.449072 | 0.028783 | 0.070302 | 0.052* |
| C     | 0.5016 (2) | −0.0234 (3) | 0.2432 (5) | 0.0392 (14) |
| H     | 0.483035 | −0.036371 | 0.0679 (10) | 0.054 (10) |
| H     | 0.425520 | −0.006979 | 0.181001 | 0.052* |
| Atom | X         | Y         | Z         | Temperature |
|------|-----------|-----------|-----------|-------------|
| O2B  | 0.39953 (9)| 0.13889 (15)| 0.9060 (2) | 0.0337 (7)  |
| O3B  | 0.36660 (9)| 0.08654 (15)| 0.7645 (2) | 0.0352 (7)  |
| N1B  | 0.45666 (10)| 0.16087 (16)| 0.5509 (2) | 0.0238 (6)  |
| H1NB | 0.4580 (11)| 0.1419 (18)| 0.478 (3)  | 0.015 (9)*  |
| C2B  | 0.42144 (11)| 0.15947 (18)| 0.7226 (3) | 0.0215 (7)  |
| C3B  | 0.44784 (11)| 0.21896 (17)| 0.7645 (3) | 0.0192 (6)  |
| H3BA | 0.455138| 0.208552| 0.843420| 0.023* |
| C4B  | 0.48650 (11)| 0.22308 (17)| 0.6980 (3) | 0.0202 (7)  |
| C5B  | 0.52170 (11)| 0.25356 (17)| 0.7503 (3) | 0.0214 (7)  |
| C6B  | 0.56081 (13)| 0.2624 (2)   | 0.6833 (3) | 0.0283 (8)  |
| C7B  | 0.55222 (14)| 0.2632 (2)   | 0.5602 (3) | 0.0353 (9)  |
| C8B  | 0.52497 (12)| 0.2027 (2)   | 0.5206 (3) | 0.0274 (8)  |
| H8BA | 0.516517| 0.211170| 0.442931| 0.033* |
| H8BB | 0.540204| 0.158121| 0.522827| 0.033* |
| C9B  | 0.48827 (12)| 0.19693 (18)| 0.5940 (3) | 0.0217 (7)  |
| H10B | 0.39848 (14)| 0.0853 (2)   | 0.5569 (3) | 0.0327 (9)  |
| H10F | 0.370242| 0.099190| 0.565137| 0.049* |
| H10E | 0.402363| 0.038514| 0.588696| 0.049* |
| C10F | 0.405593| 0.084498| 0.477890| 0.049* |
| C11B | 0.39505 (12)| 0.12824 (19)| 0.8071 (3) | 0.0249 (7)  |
| C12B | 0.34032 (15)| 0.0438 (2)   | 0.8350 (4) | 0.0408 (11) |
| C13B | 0.36627 (19)| −0.0084 (3)  | 0.8969 (5) | 0.0636 (16) |
| H13D | 0.382559| 0.016253| 0.952372| 0.095* |
| H13E | 0.384013| −0.032506| 0.844298| 0.095* |
| H13F | 0.349019| −0.042810| 0.934182| 0.095* |
| C14B | 0.31430 (18)| 0.0074 (3)   | 0.7477 (4) | 0.0605 (16) |
| H14D | 0.300055| 0.042709| 0.703607| 0.091* |
| H14E | 0.294700| −0.023052| 0.784723| 0.091* |
| H14F | 0.331456| −0.020787| 0.698874| 0.091* |
| C15B | 0.31514 (17)| 0.0884 (3)   | 0.9105 (4) | 0.0538 (14) |
| H15D | 0.332446| 0.110615| 0.966285| 0.081* |
| H15E | 0.295027| 0.059134| 0.947783| 0.081* |
| H15F | 0.301516| 0.124668| 0.866833| 0.081* |
| C16B | 0.58283 (17)| 0.3280 (3)   | 0.7172 (5) | 0.0588 (15) |
| H16D | 0.567336| 0.369113| 0.693858| 0.088* |
| H16E | 0.609364| 0.328881| 0.681709| 0.088* |
| H16F | 0.586101| 0.328634| 0.798126| 0.088* |
| C17B | 0.58741 (17)| 0.1989 (3)   | 0.7168 (4) | 0.0548 (14) |
| H17D | 0.614125| 0.203879| 0.683244| 0.082* |
| H17E | 0.574862| 0.155539| 0.690542| 0.082* |
| H17F | 0.590032| 0.197348| 0.797901| 0.082* |
| C18B | 0.42474 (11)| 0.28796 (17)| 0.7628 (3) | 0.0201 (6)  |
| C19B | 0.40710 (11)| 0.31303 (19)| 0.8600 (3) | 0.0236 (7)  |
| H19B | 0.411061| 0.288512| 0.927788| 0.028* |
| C20B | 0.38374 (12)| 0.37360 (19)| 0.8589 (3) | 0.0278 (8)  |
| H20B | 0.372096| 0.390038| 0.926144| 0.033* |
| Atom  | x    | y    | z    | U(eq) |
|-------|------|------|------|-------|
| C21B  | 0.37724 (12) | 0.41026 (19) | 0.7609 (3) | 0.0271 (8) |
| C22B  | 0.39484 (12) | 0.38486 (19) | 0.6634 (3) | 0.0270 (8) |
| H22B  | 0.390634 | 0.408871 | 0.595268 | 0.032* |
| C23B  | 0.41843 (12) | 0.32481 (18) | 0.6654 (3) | 0.0243 (7) |
| H23B  | 0.430470 | 0.308722 | 0.598470 | 0.029* |
| C24B  | 0.35100 (13) | 0.4735 (2) | 0.7599 (3) | 0.0306 (8) |
| C25B  | 0.32067 (16) | 0.4813 (3) | 0.6810 (4) | 0.0496 (12) |
| H25B  | 0.317420 | 0.446661 | 0.624996 | 0.059* |
| C26B  | 0.29521 (18) | 0.5386 (3) | 0.6827 (5) | 0.0590 (15) |
| H26B  | 0.274837 | 0.543358 | 0.627813 | 0.071* |
| C27B  | 0.29953 (17) | 0.5892 (2) | 0.7652 (4) | 0.0494 (12) |
| H27B  | 0.281795 | 0.628257 | 0.767420 | 0.059* |
| C28B  | 0.32936 (16) | 0.5828 (2) | 0.8431 (4) | 0.0449 (11) |
| H28B  | 0.332575 | 0.617497 | 0.899039 | 0.054* |
| C29B  | 0.35499 (15) | 0.5249 (2) | 0.8398 (4) | 0.0392 (10) |
| H29B  | 0.375687 | 0.520736 | 0.893877 | 0.047* |
| O1A   | 0.19045 (8) | 0.90494 (14) | 0.6522 (2) | 0.0291 (6) |
| O2A   | 0.31575 (10) | 0.77814 (17) | 0.5886 (2) | 0.0413 (8) |
| O3A   | 0.35749 (9) | 0.75149 (15) | 0.7299 (2) | 0.0327 (6) |
| N1A   | 0.27887 (10) | 0.85463 (16) | 0.9468 (2) | 0.0225 (6) |
| H1NA  | 0.2869 (14) | 0.872 (2) | 1.015 (4) | 0.034 (12)* |
| C1A   | 0.30583 (12) | 0.81797 (19) | 0.8791 (3) | 0.0234 (7) |
| C2A   | 0.29537 (11) | 0.80338 (18) | 0.7730 (3) | 0.0217 (7) |
| C3A   | 0.25278 (11) | 0.81758 (17) | 0.7316 (3) | 0.0216 (7) |
| H3AA  | 0.254555 | 0.833656 | 0.652717 | 0.026* |
| C4A   | 0.23328 (11) | 0.87495 (17) | 0.7985 (3) | 0.0201 (7) |
| C5A   | 0.20096 (11) | 0.91507 (18) | 0.7502 (3) | 0.0225 (7) |
| C6A   | 0.17859 (12) | 0.96972 (19) | 0.8190 (3) | 0.0248 (7) |
| C7A   | 0.20552 (13) | 0.9979 (2) | 0.9126 (3) | 0.0334 (9) |
| H7AA  | 0.226618 | 1.028171 | 0.879871 | 0.040* |
| H7AB  | 0.189038 | 1.027278 | 0.962894 | 0.040* |
| C8A   | 0.22563 (12) | 0.9401 (2) | 0.9804 (3) | 0.0258 (8) |
| H8AA  | 0.245670 | 0.960979 | 1.031508 | 0.031* |
| H8AB  | 0.205142 | 0.915549 | 1.025665 | 0.031* |
| C9A   | 0.24611 (12) | 0.88866 (17) | 0.9046 (3) | 0.0213 (7) |
| C10A  | 0.34394 (12) | 0.8005 (2) | 0.9392 (3) | 0.0280 (8) |
| H10A  | 0.348828 | 0.749983 | 0.934835 | 0.042* |
| H10B  | 0.341518 | 0.814513 | 1.017266 | 0.042* |
| H10C  | 0.366455 | 0.825680 | 0.904907 | 0.042* |
| C11A  | 0.32364 (12) | 0.77620 (19) | 0.6876 (3) | 0.0244 (7) |
| C12A  | 0.39117 (12) | 0.7288 (2) | 0.6574 (3) | 0.0343 (9) |
| C13A  | 0.4052 (2) | 0.7882 (3) | 0.5884 (6) | 0.082 (2) |
| H13A  | 0.385439 | 0.797594 | 0.529805 | 0.123* |
| H13B  | 0.431160 | 0.776395 | 0.554694 | 0.123* |
| H13C  | 0.408238 | 0.829931 | 0.635093 | 0.123* |
| C14A  | 0.42246 (17) | 0.7077 (5) | 0.7437 (5) | 0.086 (2) |
| H14A  | 0.434532 | 0.749834 | 0.776152 | 0.128* |
| H14B  | 0.443469 | 0.679505 | 0.708135 | 0.128* |
### Atomic Displacement Parameters (Å²)

| Atom | U₁₁      | U₂₂      | U₃₃      | U₁₂      | U₁₃      | U₂₃      |
|------|----------|----------|----------|----------|----------|----------|
| O1C  | 0.051 (2) | 0.0247 (13) | 0.0196 (12) | 0.0041 (12) | 0.0034 (12) | 0.0022 (10) |
| O2C  | 0.069 (2) | 0.0285 (14) | 0.0226 (13) | −0.0081 (15) | 0.0078 (13) | −0.0045 (11) |
| O3C  | 0.052 (2) | 0.0240 (13) | 0.0240 (13) | −0.0068 (12) | 0.0055 (12) | −0.0046 (10) |
| N1C  | 0.0224 (16) | 0.0256 (14) | 0.0149 (12) | −0.0024 (12) | 0.0018 (11) | −0.0009 (11) |
| C1C  | 0.0212 (19) | 0.0229 (16) | 0.0210 (15) | 0.0036 (14) | −0.0036 (12) | 0.0010 (12) |
| C2C  | 0.0246 (19) | 0.0239 (16) | 0.0161 (14) | 0.0031 (14) | −0.0019 (12) | −0.0019 (12) |
| C3C  | 0.0234 (18) | 0.0215 (15) | 0.0136 (13) | 0.0037 (13) | −0.0006 (12) | −0.0008 (12) |
| C4C  | 0.023 (2) | 0.0247 (16) | 0.0187 (15) | 0.0021 (14) | −0.0022 (12) | −0.0013 (12) |
| C9C  | 0.0209 (19) | 0.0270 (17) | 0.0168 (14) | 0.0012 (14) | −0.0027 (12) | −0.0021 (12) |
| C10C | 0.035 (2) | 0.0270 (17) | 0.0223 (16) | −0.0047 (16) | 0.0009 (15) | 0.0011 (14) |

*sup-6*
| Atom  | U1     | U2     | U3     | U4     | U5     | U6     |
|-------|--------|--------|--------|--------|--------|--------|
| C11C  | 0.034  | 0.0207 | 0.0205 | 0.0028 | 0.0010 | −0.0016|
| C12C  | 0.053  | 0.0259 | 0.0297 | −0.0027| 0.0014 | −0.0097|
| C13C  | 0.053  | 0.045  | 0.061  | 0.006  | −0.017 | −0.021 |
| C14C  | 0.110  | 0.035  | 0.045  | −0.030 | 0.015  | −0.012 |
| C15C  | 0.051  | 0.034  | 0.052  | 0.000  | −0.004 | −0.017 |
| C5C   | 0.017  | 0.021  | 0.017  | −0.002 | 0.005  | 0.001  |
| C6C   | 0.028  | 0.0228 | 0.019  | 0.004  | −0.002 | −0.002 |
| C7C   | 0.029  | 0.022  | 0.026  | 0.003  | 0.001  | −0.0031|
| C8C   | 0.028  | 0.0290 | 0.009  | 0.0022 | 0.005  | −0.0020|
| C16C  | 0.042  | 0.030  | 0.032  | 0.001  | 0.002  | −0.009 |
| C17C  | 0.058  | 0.033  | 0.027  | 0.020  | −0.002 | −0.003 |
| C5F   | 0.017  | 0.021  | 0.017  | −0.002 | 0.005  | 0.001  |
| C6F   | 0.028  | 0.0228 | 0.019  | 0.004  | −0.002 | −0.002 |
| C7F   | 0.029  | 0.022  | 0.006  | 0.003  | 0.001  | −0.0031|
| C8F   | 0.028  | 0.0290 | 0.009  | 0.0022 | 0.005  | −0.0020|
| C16F  | 0.042  | 0.030  | 0.032  | 0.001  | 0.002  | −0.009 |
| C17F  | 0.058  | 0.033  | 0.027  | 0.020  | −0.002 | −0.003 |
| C18C  | 0.0265 | 0.0162 | 0.0189 | 0.0028 | 0.0046 | 0.0023 |
| C19C  | 0.033  | 0.0301 | 0.0229 | 0.0065 | 0.0063 | 0.0023 |
| C20C  | 0.031  | 0.037  | 0.032  | 0.0077 | 0.0126 | 0.0007 |
| C21C  | 0.026  | 0.0271 | 0.041  | 0.0035 | 0.0062 | 0.0057 |
| C22C  | 0.024  | 0.035  | 0.032  | −0.0013| −0.0020| 0.0040 |
| C23C  | 0.025  | 0.0289 | 0.0231 | −0.0002| 0.0003 | 0.0007 |
| C24C  | 0.026  | 0.044  | 0.054  | 0.0030 | 0.0069 | 0.012  |
| C25C  | 0.034  | 0.071  | 0.099  | 0.014  | 0.014  | −0.007 |
| C26C  | 0.035  | 0.084  | 0.126  | 0.016  | 0.021  | 0.003  |
| C27C  | 0.024  | 0.084  | 0.116  | 0.011  | 0.006  | 0.031  |
| C28C  | 0.035  | 0.082  | 0.082  | −0.003 | −0.005 | 0.031  |
| C29C  | 0.031  | 0.059  | 0.063  | −0.003 | −0.001 | 0.017  |
| C1B   | 0.026  | 0.0222 | 0.0201 | 0.0013 | −0.0041| 0.0027 |
| O1B   | 0.0243 | 0.0471 | 0.0189 | −0.0089| 0.0020 | −0.0034|
| O2B   | 0.0311 | 0.0481 | 0.0200 | −0.0136| 0.0004 | −0.0024|
| O3B   | 0.0350 | 0.0450 | 0.0257 | −0.0183| 0.0066 | −0.0055|
| N1B   | 0.0297 | 0.0278 | 0.0139 | −0.0022| −0.0001| −0.0024|
| C2B   | 0.0207 | 0.0262 | 0.0176 | 0.0014 | −0.0003| 0.0002 |
| C3B   | 0.0215 | 0.0222 | 0.0140 | −0.0055| −0.0007| 0.0008 |
| C4B   | 0.0200 | 0.0220 | 0.0187 | 0.0037 | 0.0012 | 0.0027 |
| C5B   | 0.0205 | 0.0240 | 0.0198 | 0.0010 | 0.0025 | 0.0043 |
| C6B   | 0.030  | 0.0313 | 0.0232 | −0.0034| 0.0063 | −0.0010|
| C7B   | 0.032  | 0.042  | 0.031  | −0.0033| 0.0056 | 0.0034 |
| C8B   | 0.025  | 0.038  | 0.0189 | 0.0042 | 0.0052 | −0.0001|
| C9B   | 0.026  | 0.0226 | 0.0160 | 0.0043 | 0.0009 | 0.0024 |
| C10B  | 0.035  | 0.036  | 0.0268 | −0.0076| −0.0038| −0.0062|
| C11B  | 0.022  | 0.0288 | 0.0237 | −0.0002| 0.0001 | −0.0028|
| C12B  | 0.044  | 0.043  | 0.035  | −0.025 | 0.0019 | 0.0035 |
| C13B  | 0.065  | 0.048  | 0.078  | −0.016 | 0.009  | 0.020  |
| C14B  | 0.059  | 0.073  | 0.050  | −0.044 | 0.014  | −0.018 |
| C15B  | 0.044  | 0.072  | 0.046  | −0.023 | 0.020  | −0.005 |
| Atom | U11 | U22 | U33 | U12 | U13 | U23 |
|------|-----|-----|-----|-----|-----|-----|
| C16B | 0.038 (3) | 0.056 (3) | -0.022 (3) | 0.014 (2) | -0.004 (3) |
| C17B | 0.045 (3) | 0.036 (3) | -0.020 (3) | 0.002 (2) | 0.009 (2) |
| C18B | 0.0179 (17) | 0.0008 (13) | -0.0030 (12) | -0.0010 (12) |
| C19B | 0.023 (2) | 0.0190 (14) | 0.0006 (12) | -0.0004 (13) |
| C20B | 0.026 (2) | 0.0046 (16) | -0.0028 (14) | -0.0054 (14) |
| C21B | 0.0221 (19) | 0.0031 (14) | -0.0003 (15) | 0.0012 (15) |
| C22B | 0.027 (2) | 0.0056 (16) | 0.0012 (14) | 0.0012 (14) |
| C23B | 0.026 (2) | 0.0041 (15) | 0.0021 (13) | -0.0009 (13) |
| C24B | 0.029 (2) | 0.0077 (16) | 0.0048 (16) | 0.0023 (16) |
| C25B | 0.040 (3) | 0.011 (2) | -0.007 (2) | -0.001 (2) |
| C26B | 0.040 (3) | 0.021 (3) | -0.009 (3) | 0.001 (3) |
| C27B | 0.043 (3) | 0.017 (2) | 0.008 (2) | 0.001 (2) |
| C28B | 0.052 (3) | 0.008 (2) | 0.015 (2) | -0.0005 (19) |
| C29B | 0.040 (3) | 0.0089 (19) | 0.009 (2) | 0.0032 (18) |
| O1A | 0.02063 (15) | 0.0097 (12) | -0.0028 (10) | -0.0048 (11) |
| O2A | 0.02034 (18) | 0.0237 (16) | 0.0006 (11) | -0.0042 (13) |
| O3A | 0.02021 (15) | 0.0112 (13) | 0.0013 (10) | -0.0044 (12) |
| N1A | 0.02064 (17) | -0.0003 (13) | -0.0024 (11) | -0.0015 (11) |
| C1A | 0.0324 (2) | -0.0025 (15) | -0.0002 (12) | 0.0023 (12) |
| C2A | 0.02017 (19) | 0.0023 (14) | 0.0000 (12) | -0.0027 (13) |
| C3A | 0.02018 (18) | 0.0028 (14) | 0.0011 (12) | -0.0007 (12) |
| C4A | 0.02025 (19) | 0.0018 (14) | 0.0018 (12) | -0.0013 (12) |
| C5A | 0.02026 (19) | 0.0004 (14) | 0.0015 (13) | -0.0008 (12) |
| C6A | 0.02025 (2) | 0.0063 (15) | 0.0007 (13) | -0.0014 (13) |
| C7A | 0.0323 (19) | 0.0028 (18) | 0.0019 (16) | -0.0064 (16) |
| C8A | 0.02026 (2) | 0.0006 (16) | 0.0022 (13) | -0.0072 (14) |
| C9A | 0.02024 (19) | -0.0021 (14) | 0.0027 (12) | -0.0017 (12) |
| C10A | 0.02023 (2) | 0.0038 (16) | -0.0018 (14) | -0.0011 (15) |
| C11A | 0.020205 (19) | 0.0027 (15) | -0.0003 (13) | -0.0020 (13) |
| C12A | 0.0164 (19) | 0.0097 (18) | 0.0023 (14) | -0.0045 (18) |
| C13A | 0.058 (4) | 0.008 (3) | 0.055 (4) | 0.021 (4) |
| C14A | 0.030 (3) | 0.045 (4) | -0.011 (2) | -0.028 (4) |
| C15A | 0.035 (3) | 0.013 (3) | 0.010 (2) | -0.025 (3) |
| C16A | 0.036 (3) | 0.000 (2) | 0.0089 (19) | -0.0111 (19) |
| C17A | 0.035 (2) | 0.014 (2) | -0.002 (2) | -0.003 (2) |
| C18A | 0.0194 (18) | 0.0031 (14) | -0.0036 (12) | -0.0006 (12) |
| C19A | 0.029 (2) | -0.0026 (15) | -0.0019 (14) | -0.0017 (13) |
| C20A | 0.033 (2) | 0.0047 (16) | -0.0043 (15) | -0.0067 (14) |
| C21A | 0.024 (2) | 0.00252 (14) | -0.0006 (14) | -0.0020 (14) |
| C22A | 0.029 (2) | -0.0005 (17) | 0.0003 (15) | 0.0006 (15) |
| C23A | 0.027 (2) | 0.0003 (16) | -0.0011 (13) | -0.0038 (13) |
| C24A | 0.029 (2) | 0.0008 (16) | 0.0068 (16) | -0.0031 (16) |
| C25A | 0.048 (3) | 0.007 (2) | -0.003 (2) | 0.005 (2) |
| C26A | 0.068 (4) | 0.005 (3) | 0.010 (3) | 0.012 (2) |
| C27A | 0.050 (3) | 0.008 (2) | 0.012 (2) | -0.006 (2) |
| C28A | 0.049 (3) | 0.011 (2) | 0.013 (2) | -0.016 (2) |
| C29A | 0.044 (3) | 0.006 (2) | 0.006 (2) | -0.0079 (19) |
Geometric parameters (Å, °)

| Bond                  | Length  | Angle       |
|-----------------------|---------|-------------|
| O1C—C5F               | 1.11(4) | C10B—H10D  | 0.9800 |
| O1C—C5C               | 1.282(12)| C10B—H10E | 0.9800 |
| O2C—C11C              | 1.219(4) | C10B—H10F | 0.9800 |
| O3C—C11C              | 1.332(4) | C12B—C15B | 1.501(7) |
| O3C—C12C              | 1.468(4) | C12B—C13B | 1.514(7) |
| N1C—C9C               | 1.363(4) | C12B—C14B | 1.528(6) |
| N1C—C1C               | 1.392(4) | C13B—H13D | 0.9800 |
| N1C—H1NC              | 0.92(5)  | C13B—H13E | 0.9800 |
| C1C—C2C               | 1.351(5) | C13B—H13F | 0.9800 |
| C1C—C10C              | 1.495(5) | C14B—H14D | 0.9800 |
| C2C—C11C              | 1.474(5) | C14B—H14E | 0.9800 |
| C2C—C3C               | 1.519(5) | C14B—H14F | 0.9800 |
| C3C—C18C              | 1.518(5) | C15B—H15D | 0.9800 |
| C3C—C4C               | 1.523(5) | C15B—H15E | 0.9800 |
| C3C—H3CA              | 1.0000  | C15B—H15F | 0.9800 |
| C4C—C9C               | 1.352(5) | C16B—H16D | 0.9800 |
| C4C—C5C               | 1.416(13)| C16B—H16E | 0.9800 |
| C4C—C5F               | 1.57(3)  | C16B—H16F | 0.9800 |
| C9C—C8F               | 1.41(4)  | C17B—H17D | 0.9800 |
| C9C—C8C               | 1.537(15)| C17B—H17E | 0.9800 |
| C10C—H11G             | 0.9800  | C17B—H17F | 0.9800 |
| C10C—H10H             | 0.9800  | C18B—C23B | 1.384(5) |
| C10C—H10I             | 0.9800  | C18B—C19B | 1.393(5) |
| C12C—C15C             | 1.507(6) | C19B—C20B | 1.393(5) |
| C12C—C13C             | 1.518(7) | C19B—H19B | 0.9500 |
| C12C—C14C             | 1.519(6) | C20B—C21B | 1.389(5) |
| C13C—H13G             | 0.9800  | C20B—H20B | 0.9500 |
| C13C—H13H             | 0.9800  | C21B—C22B | 1.398(5) |
| C13C—H13I             | 0.9800  | C21B—C24B | 1.488(5) |
| C14C—H14G             | 0.9800  | C22B—C23B | 1.389(5) |
| C14C—H14H             | 0.9800  | C22B—H22B | 0.9500 |
| C14C—H14I             | 0.9800  | C23B—H23B | 0.9500 |
| C15C—H15G             | 0.9800  | C24B—C29B | 1.381(6) |
| C15C—H15H             | 0.9800  | C24B—C25B | 1.393(6) |
| C15C—H15I             | 0.9800  | C25B—C26B | 1.383(7) |
| C5C—C6C               | 1.543(8) | C25B—H25B | 0.9500 |
| C6C—C16C              | 1.529(8) | C26B—C27B | 1.394(7) |
| C6C—C17C              | 1.534(8) | C26B—H26B | 0.9500 |
| C6C—C7C               | 1.534(9) | C27B—C28B | 1.370(7) |
| C7C—C8C               | 1.514(13)| C27B—H27B | 0.9500 |
| C7C—H7CA              | 0.9900  | C28B—C29B | 1.396(6) |
| C7C—H7CB              | 0.9900  | C28B—H28B | 0.9500 |
| C8C—H8CA              | 0.9900  | C29B—H29B | 0.9500 |
| C8C—H8CB              | 0.9900  | O1A—C5A   | 1.246(4) |
| C16C—H16G             | 0.9800  | O2A—C11A  | 1.221(4) |
| C16C—H16H             | 0.9800  | O3A—C11A  | 1.322(5) |
| Bond                | Distance (Å) | Bond                | Distance (Å) |
|---------------------|--------------|---------------------|--------------|
| C16C—H16I          | 0.9800       | O3A—C12A            | 1.483 (5)    |
| C17C—H17G          | 0.9800       | N1A—C9A             | 1.365 (5)    |
| C17C—H17H          | 0.9800       | N1A—C1A             | 1.398 (5)    |
| C17C—H17I          | 0.9800       | N1A—H1NA            | 0.92 (4)     |
| C5F—C6F            | 1.548 (18)   | C1A—C2A             | 1.533 (5)    |
| C6F—C16F           | 1.526 (19)   | C1A—C10A            | 1.496 (5)    |
| C6F—C7F            | 1.530 (17)   | C2A—C11A            | 1.486 (5)    |
| C6F—C17F           | 1.547 (19)   | C2A—C3A             | 1.525 (5)    |
| C7F—C8F            | 1.52 (2)     | C3A—C4A             | 1.506 (5)    |
| C7F—H7FA           | 0.9900       | C3A—C18A            | 1.527 (5)    |
| C7F—H7FB           | 0.9900       | C3A—H3AA            | 1.0000       |
| C8F—H8FA           | 0.9900       | C4A—C9A             | 1.372 (5)    |
| C8F—H8FB           | 0.9900       | C4A—C5A             | 1.442 (5)    |
| C16F—H16J          | 0.9800       | C5A—C6A             | 1.525 (5)    |
| C16F—H16K          | 0.9800       | C6A—C17A            | 1.518 (6)    |
| C16F—H16L          | 0.9800       | C6A—C16A            | 1.535 (6)    |
| C17F—H17J          | 0.9800       | C6A—C7A             | 1.537 (5)    |
| C17F—H17K          | 0.9800       | C7A—C8A             | 1.527 (6)    |
| C17F—H17L          | 0.9800       | C7A—H7AA            | 0.9900       |
| C18C—C23C          | 1.398 (5)    | C7A—H7AB            | 0.9900       |
| C18C—C19C          | 1.399 (5)    | C8A—C9A             | 1.503 (5)    |
| C19C—C20C          | 1.389 (6)    | C8A—H8AA            | 0.9900       |
| C19C—H19C          | 0.9500       | C8A—H8AB            | 0.9900       |
| C20C—C21C          | 1.387 (6)    | C10A—H10A           | 0.9800       |
| C20C—H20C          | 0.9500       | C10A—H10B           | 0.9800       |
| C21C—C22C          | 1.394 (6)    | C10A—H10C           | 0.9800       |
| C21C—C24C          | 1.487 (6)    | C12A—C13A           | 1.480 (7)    |
| C22C—C23C          | 1.377 (6)    | C12A—C15A           | 1.488 (7)    |
| C22C—H22C          | 0.9500       | C12A—C14A           | 1.524 (7)    |
| C23C—H23C          | 0.9500       | C13A—H13A           | 0.9800       |
| C24C—C25C          | 1.387 (7)    | C13A—H13B           | 0.9800       |
| C24C—C29C          | 1.411 (7)    | C13A—H13C           | 0.9800       |
| C25C—C26C          | 1.382 (9)    | C14A—H14A           | 0.9800       |
| C25C—H25C          | 0.9500       | C14A—H14B           | 0.9800       |
| C26C—C27C          | 1.374 (10)   | C14A—H14C           | 0.9800       |
| C26C—H26C          | 0.9500       | C15A—H15A           | 0.9800       |
| C27C—C28C          | 1.400 (9)    | C15A—H15B           | 0.9800       |
| C27C—H27C          | 0.9500       | C15A—H15C           | 0.9800       |
| C28C—C29C          | 1.399 (8)    | C16A—H16A           | 0.9800       |
| C28C—H28C          | 0.9500       | C16A—H16B           | 0.9800       |
| C29C—H29C          | 0.9500       | C16A—H16C           | 0.9800       |
| C1B—C2B            | 1.354 (5)    | C17A—H17A           | 0.9800       |
| C1B—N1B            | 1.397 (5)    | C17A—H17B           | 0.9800       |
| C1B—C10B           | 1.500 (5)    | C17A—H17C           | 0.9800       |
| O1B—C5B            | 1.235 (4)    | C18A—C23A           | 1.387 (5)    |
| O2B—C11B           | 1.216 (4)    | C18A—C19A           | 1.402 (5)    |
| O3B—C11B           | 1.338 (5)    | C19A—C20A           | 1.395 (5)    |
| O3B—C12B           | 1.466 (5)    | C19A—H19A           | 0.9500       |
| Bond | Length (Å) | Bond | Length (Å) | Bond | Length (Å) |
|------|------------|------|------------|------|------------|
| N1B—C9B | 1.358 (5) | C20A—C21A | 1.384 (5) |
| N1B—H1NB | 0.95 (4) | C20A—H20A | 0.9500 |
| C2B—C11B | 1.469 (5) | C21A—C22A | 1.389 (5) |
| C2B—C3B | 1.521 (5) | C21A—C24A | 1.499 (5) |
| C2B—C4B | 1.515 (5) | C22A—C23A | 1.392 (5) |
| C3B—C18B | 1.525 (5) | C22A—H22A | 0.9500 |
| C3B—H3BA | 1.0000 | C23A—H23A | 0.9500 |
| C4B—C9B | 1.350 (5) | C24A—C25A | 1.387 (6) |
| C4B—C5B | 1.450 (5) | C24A—C29A | 1.399 (6) |
| C5B—C6B | 1.538 (5) | C25A—C26A | 1.393 (7) |
| C6B—C16B | 1.507 (7) | C25A—H25A | 0.9500 |
| C6B—C7B | 1.510 (5) | C26A—C27A | 1.369 (8) |
| C6B—C17B | 1.553 (7) | C26A—H26A | 0.9500 |
| C7B—C8B | 1.543 (6) | C27A—C28A | 1.373 (7) |
| C7B—H7BA | 0.9900 | C27A—H27A | 0.9500 |
| C7B—H7BB | 0.9900 | C28A—C29A | 1.384 (6) |
| C8B—C9B | 1.509 (5) | C28A—H28A | 0.9500 |
| C8B—H8BA | 0.9900 | C29A—H29A | 0.9500 |
| C8B—H8BB | 0.9900 |

| Bond | Angle (°) | Bond | Angle (°) | Bond | Angle (°) |
|------|----------|------|----------|------|----------|
| C11C—O3C—C12C | 122.1 (3) | C1B—C10B—H10E | 109.5 |
| C9C—N1C—C1C | 122.2 (3) | H10D—C10B—H10E | 109.5 |
| C9C—N1C—H1NC | 123 (3) | C1B—C10B—H10F | 109.5 |
| C1C—N1C—H1NC | 113 (3) | H10D—C10B—H10F | 109.5 |
| C2C—C1C—N1C | 119.1 (3) | C1B—C10B—H10F | 109.5 |
| C2C—C1C—C10C | 128.3 (3) | O2B—C11B—O3B | 124.1 (4) |
| N1C—C1C—C10C | 112.5 (3) | O2B—C11B—C2B | 122.4 (4) |
| C1C—C2C—C11C | 124.7 (3) | O3B—C11B—C2B | 113.4 (3) |
| C1C—C2C—C3C | 120.4 (3) | O3B—C12B—C15B | 111.5 (4) |
| C11C—C2C—C3C | 114.9 (3) | O3B—C12B—C13B | 108.2 (4) |
| C18C—C3C—C2C | 111.1 (3) | O3B—C12B—C13B | 113.1 (4) |
| C18C—C3C—C4C | 112.5 (3) | O3B—C12B—C14B | 101.1 (3) |
| C2C—C3C—C4C | 109.3 (3) | C15B—C12B—C14B | 111.1 (4) |
| C18C—C3C—H3CA | 107.9 | C13B—C12B—C14B | 111.2 (4) |
| C2C—C3C—H3CA | 107.9 | C12B—C13B—H13D | 109.5 |
| C4C—C3C—H3CA | 107.9 | C12B—C13B—H13E | 109.5 |
| C9C—C4C—C5C | 119.4 (5) | H13D—C13B—H13E | 109.5 |
| C9C—C4C—C3C | 120.3 (3) | C12B—C13B—H13F | 109.5 |
| C5C—C4C—C3C | 120.3 (4) | H13D—C13B—H13F | 109.5 |
| C9C—C4C—C5F | 124.6 (9) | H13E—C13B—H13F | 109.5 |
| C3C—C4C—C5F | 114.6 (9) | C12B—C14B—H14D | 109.5 |
| C4C—C9C—N1C | 120.0 (3) | C12B—C14B—H14E | 109.5 |
| C4C—C9C—C8F | 118.8 (10) | H14D—C14B—H14E | 109.5 |
| N1C—C9C—C8F | 121.2 (10) | C12B—C14B—H14F | 109.5 |
| C4C—C9C—C8C | 125.4 (4) | H14D—C14B—H14F | 109.5 |
| N1C—C9C—C8C | 114.5 (4) | H14E—C14B—H14F | 109.5 |
| C1C—C10C—H10G | 109.5 | C12B—C15B—H15D | 109.5 |
| C1C—C10C—H10H | 109.5 | C12B—C15B—H15E | 109.5 |
| Bond | Angle | Bond | Angle | Bond | Angle |
|------|-------|------|-------|------|-------|
| H10G—C10C—H10H | 109.5 | H15D—C15B—H15E | 109.5 |
| C1C—C10C—H10I | 109.5 | C12B—C15B—H15F | 109.5 |
| H10G—C10C—H10I | 109.5 | H15D—C15B—H15F | 109.5 |
| H10H—C10C—H10I | 109.5 | H15E—C15B—H15F | 109.5 |
| O2C—C11C—O3C | 123.9 (3) | C6B—C16B—H16D | 109.5 |
| O2C—C11C—C2C | 122.6 (3) | C6B—C16B—H16E | 109.5 |
| O3C—C11C—C2C | 113.5 (3) | H16D—C16B—H16E | 109.5 |
| O3C—C12C—C15C | 109.9 (4) | C6B—C16B—H16F | 109.5 |
| O3C—C12C—C13C | 110.2 (3) | H16D—C16B—H16F | 109.5 |
| C15C—C12C—C13C | 112.8 (4) | H16E—C16B—H16F | 109.5 |
| O3C—C12C—C14C | 101.7 (3) | C6B—C17B—H17D | 109.5 |
| C15C—C12C—C14C | 111.0 (4) | C6B—C17B—H17E | 109.5 |
| C13C—C12C—C14C | 110.6 (5) | H17D—C17B—H17E | 109.5 |
| C12C—C13C—H13G | 109.5 | C6B—C17B—H17F | 109.5 |
| C12C—C13C—H13H | 109.5 | H17D—C17B—H17F | 109.5 |
| H13G—C13C—H13H | 109.5 | H17E—C17B—H17F | 109.5 |
| C12C—C13C—H13I | 109.5 | C23B—C18B—C19B | 118.3 (3) |
| H13G—C13C—H13I | 109.5 | C23B—C18B—C3B | 121.8 (3) |
| H13H—C13C—H13I | 109.5 | C19B—C18B—C3B | 119.8 (3) |
| C12C—C14C—H14G | 109.5 | C18B—C19B—C20B | 120.8 (3) |
| C12C—C14C—H14H | 109.5 | C18B—C19B—H19B | 119.6 |
| H14G—C14C—H14H | 109.5 | C20B—C19B—H19B | 119.6 |
| C12C—C14C—H14I | 109.5 | C21B—C20B—C19B | 120.9 (3) |
| H14G—C14C—H14I | 109.5 | C21B—C20B—H20B | 119.6 |
| H14H—C14C—H14I | 109.5 | C19B—C20B—H20B | 119.6 |
| C12C—C15C—H15G | 109.5 | C20B—C21B—C22B | 118.2 (3) |
| C12C—C15C—H15H | 109.5 | C20B—C21B—C24B | 120.5 (3) |
| H15G—C15C—H15H | 109.5 | C22B—C21B—C24B | 121.2 (3) |
| C12C—C15C—H15I | 109.5 | C23B—C22B—C21B | 120.5 (3) |
| H15G—C15C—H15I | 109.5 | C23B—C22B—H22B | 119.7 |
| H15H—C15C—H15I | 109.5 | C21B—C22B—H22B | 119.7 |
| O1C—C5C—C4C | 121.1 (6) | C18B—C23B—C22B | 121.3 (3) |
| O1C—C5C—C6C | 118.3 (8) | C18B—C23B—H23B | 119.4 |
| C4C—C5C—C6C | 119.5 (9) | C22B—C23B—H23B | 119.4 |
| C16C—C6C—C17C | 109.5 (6) | C29B—C24B—C25B | 117.9 (4) |
| C16C—C6C—C7C | 111.1 (5) | C29B—C24B—C21B | 120.9 (4) |
| C17C—C6C—C7C | 110.0 (6) | C25B—C24B—C21B | 121.1 (4) |
| C16C—C6C—C5C | 108.4 (7) | C26B—C25B—C24B | 121.2 (5) |
| C17C—C6C—C5C | 109.4 (7) | C26B—C25B—H25B | 119.4 |
| C7C—C6C—C5C | 108.4 (6) | C24B—C25B—H25B | 119.4 |
| C8C—C7C—C6C | 113.2 (8) | C25B—C26B—C27B | 119.8 (5) |
| C8C—C7C—H7CA | 108.9 | C25B—C26B—H26B | 120.1 |
| C6C—C7C—H7CA | 108.9 | C27B—C26B—H26B | 120.1 |
| C8C—C7C—H7CB | 108.9 | C28B—C27B—C26B | 120.0 (4) |
| C6C—C7C—H7CB | 108.9 | C28B—C27B—H27B | 120.0 |
| H7CA—C7C—H7CB | 107.7 | C26B—C27B—H27B | 120.0 |
| C7C—C8C—C9C | 109.1 (8) | C27B—C28B—C29B | 119.5 (5) |
| C7C—C8C—H8CA | 109.9 | C27B—C28B—H28B | 120.2 |
C9C—C8C—H8CA 109.9  C29B—C28B—H28B 120.2  
C7C—C8C—H8CB 109.9  C24B—C29B—C28B 121.6 (5)  
C9C—C8C—H8CB 109.9  C24B—C29B—H29B 119.2  
H8CA—C8C—H8CB 108.3  C28B—C29B—H29B 119.2  
C6C—C16C—C16G 109.5  C11A—O3A—C12A 121.3 (3)  
C6C—C16C—C16H 109.5  C9A—N1A—C1A 122.2 (3)  
H16G—C16C—H16H 109.5  C9A—N1A—H1NA 113 (3)  
C6C—C16C—H16I 109.5  C1A—N1A—H1NA 121 (3)  
H16G—C16C—H16I 109.5  C2A—C1A—N1A 119.2 (3) 
H16H—C16C—H16I 109.5  C2A—C1A—C10A 128.9 (3)   
C6C—C17C—H17G 109.5  N1A—C1A—C10A 111.8 (3)  
C6C—C17C—H17H 109.5  C1A—C2A—C11A 124.3 (3)  
H17G—C17C—H17H 109.5  C1A—C2A—C3A 120.7 (3)  
C6C—C17C—C17I 109.5  C11A—C2A—C3A 115.0 (3) 
C6C—C17C—H17I 109.5  C4A—C3A—C2A 110.7 (3) 
H17H—C17C—H17I 109.5  C4A—C3A—C18A 112.9 (3) 
O1C—C5F—C6F 120 (3)  C2A—C3A—C18A 108.8 (3) 
O1C—C5F—C4C 121.6 (19)  C4A—C3A—H3AA 108.1 
C6F—C5F—C6F 113 (2)  C2A—C3A—H3AA 108.1 
C16F—C6F—C7F 109.8 (14)  C18A—C3A—H3AA 108.1 
C16F—C6F—C17F 109.4 (14)  C9A—C4A—C5A 120.4 (3)  
C7F—C6F—C17F 112.4 (14)  C9A—C4A—C3A 120.2 (3) 
C16F—C6F—C5F 105.7 (17)  C5A—C4A—C3A 119.4 (3) 
C7F—C6F—C5F 109.8 (19)  O1A—C5A—C4A 120.6 (3) 
C17F—C6F—C5F 109.5 (19)  O1A—C5A—C6A 118.9 (3) 
C8F—C7F—C6F 112 (2)  C4A—C5A—C6A 120.5 (3) 
C8F—C7F—H7FA 109.3  C17A—C6A—C5A 111.0 (3) 
C6F—C7F—H7FA 109.3  C17A—C6A—C16A 110.1 (4) 
C8F—C7F—H7FB 109.3  C5A—C6A—C16A 106.5 (3) 
C6F—C7F—H7FB 109.3  C17A—C6A—C7A 108.8 (3) 
H7FA—C7F—H7FB 107.9  C5A—C6A—C7A 110.7 (3) 
C9C—C8F—C7F 119 (3)  C16A—C6A—C7A 109.7 (3) 
C9C—C8F—H8FA 107.5  C8A—C7A—C6A 113.2 (3) 
C7F—C8F—H8FA 107.5  C8A—C7A—H7AA 108.9 
C9C—C8F—H8FB 107.5  C6A—C7A—H7AA 108.9 
C7F—C8F—H8FB 107.5  C8A—C7A—H7AB 108.9 
H8FA—C8F—H8FB 107.0  C6A—C7A—H7AB 108.9 
C6F—C16F—H16J 109.5  H7AA—C7A—H7AB 107.8 
C6F—C16F—H16K 109.5  C9A—C8A—C7A 110.3 (3) 
H16J—C16F—H16K 109.5  C9A—C8A—H8AA 109.6 
C6F—C16F—H16L 109.5  C7A—C8A—H8AA 109.6 
H16J—C16F—H16L 109.5  C9A—C8A—H8AB 109.6 
H16K—C16F—H16L 109.5  C7A—C8A—H8AB 109.6 
C6F—C17F—H17J 109.5  H8AA—C8A—H8AB 108.1 
C6F—C17F—H17K 109.5  N1A—C9A—C4A 120.2 (3) 
H17J—C17F—H17K 109.5  N1A—C9A—C8A 116.5 (3) 
C6F—C17F—H17L 109.5  C4A—C9A—C8A 123.3 (3) 
H17J—C17F—H17L 109.5  C1A—C10A—H10A 109.5
| Bond             | Length (Å) | Bond             | Length (Å) |
|------------------|------------|------------------|------------|
| H17K—C17F—H17L  | 109.5      | C1A—C10A—H10B   | 109.5      |
| C23C—C18C—C19C  | 117.8 (3)  | H10A—C10A—H10B  | 109.5      |
| C23C—C18C—C3C   | 120.9 (3)  | C1A—C10A—H10C   | 109.5      |
| C19C—C18C—C3C   | 121.2 (3)  | H10A—C10A—H10C  | 109.5      |
| C20C—C19C—C18C  | 120.8 (4)  | H10B—C10A—H10C  | 109.5      |
| C20C—C19C—H19C  | 119.6      | O2A—C11A—O3A    | 124.7 (3)  |
| C18C—C19C—H19C  | 119.6      | O2A—C11A—C2A    | 122.0 (3)  |
| C21C—C20C—C19C  | 121.3 (4)  | O3A—C11A—C2A    | 113.3 (3)  |
| C21C—C20C—H20C  | 119.4      | C13A—C12A—O3A   | 110.1 (4)  |
| C19C—C20C—H20C  | 119.4      | C13A—C12A—C15A  | 112.6 (5)  |
| C20C—C21C—C22C  | 117.7 (4)  | O3A—C12A—C15A   | 110.9 (4)  |
| C20C—C21C—C24C  | 121.0 (4)  | C13A—C12A—C14A  | 111.8 (5)  |
| C22C—C21C—C24C  | 121.3 (4)  | O3A—C12A—C14A   | 101.0 (3)  |
| C23C—C22C—C21C  | 121.6 (4)  | C15A—C12A—C14A  | 109.9 (5)  |
| C23C—C22C—H22C  | 119.2      | C12A—C13A—H13A  | 109.5      |
| C21C—C22C—H22C  | 119.2      | C12A—C13A—H13B  | 109.5      |
| C22C—C23C—C18C  | 120.8 (4)  | H13A—C13A—H13B  | 109.5      |
| C22C—C23C—H23C  | 119.6      | C12A—C13A—H13C  | 109.5      |
| C18C—C23C—H23C  | 119.6      | H13A—C13A—H13C  | 109.5      |
| C25C—C24C—C29C  | 118.3 (5)  | H13B—C13A—H13C  | 109.5      |
| C25C—C24C—C21C  | 121.4 (5)  | C12A—C14A—H14A  | 109.5      |
| C29C—C24C—C21C  | 120.3 (4)  | C12A—C14A—H14B  | 109.5      |
| C26C—C25C—C24C  | 121.6 (7)  | H14A—C14A—H14B  | 109.5      |
| C26C—C25C—H25C  | 119.2      | C12A—C14A—H14C  | 109.5      |
| C24C—C25C—H25C  | 119.2      | H14A—C14A—H14C  | 109.5      |
| C27C—C26C—C25C  | 120.1 (6)  | H14B—C14A—H14C  | 109.5      |
| C27C—C26C—H26C  | 120.0      | C12A—C15A—H15A  | 109.5      |
| C25C—C26C—H26C  | 120.0      | C12A—C15A—H15B  | 109.5      |
| C26C—C27C—C28C  | 120.3 (6)  | H15A—C15A—H15B  | 109.5      |
| C26C—C27C—H27C  | 119.9      | C12A—C15A—H15C  | 109.5      |
| C28C—C27C—H27C  | 119.9      | H15A—C15A—H15C  | 109.5      |
| C29C—C28C—C27C  | 119.5 (6)  | H15B—C15A—H15C  | 109.5      |
| C29C—C28C—H28C  | 120.3      | C6A—C16A—H16A   | 109.5      |
| C27C—C28C—H28C  | 120.3      | C6A—C16A—H16B   | 109.5      |
| C28C—C29C—C24C  | 120.2 (6)  | H16A—C16A—H16B  | 109.5      |
| C28C—C29C—H29C  | 119.9      | C6A—C16A—H16C   | 109.5      |
| C24C—C29C—H29C  | 119.9      | H16A—C16A—H16C  | 109.5      |
| C2B—C1B—N1B     | 119.4 (3)  | H16B—C16A—H16C  | 109.5      |
| C2B—C1B—C10B    | 127.8 (4)  | C6A—C17A—H17A   | 109.5      |
| N1B—C1B—C10B    | 112.8 (3)  | C6A—C17A—H17B   | 109.5      |
| C11B—O3B—C12B   | 122.0 (3)  | H17A—C17A—H17B  | 109.5      |
| C9B—N1B—C1B     | 122.4 (3)  | C6A—C17A—H17C   | 109.5      |
| C9B—N1B—H1NB    | 121.2      | H17A—C17A—H17C  | 109.5      |
| C1B—N1B—H1NB    | 115.2      | H17B—C17A—H17C  | 109.5      |
| C1B—C2B—C11B    | 125.0 (3)  | C23A—C18A—C19A  | 118.2 (3)  |
| C1B—C2B—C3B     | 120.2 (3)  | C23A—C18A—C3A   | 121.4 (3)  |
| C11B—C2B—C3B    | 114.7 (3)  | C19A—C18A—C3A   | 120.3 (3)  |
| C4B—C3B—C2B     | 110.6 (3)  | C20A—C19A—C18A  | 120.3 (3)  |
C4B—C3B—C18B 112.0 (3) C20A—C19A—H19A 119.9
C2B—C3B—C18B 110.5 (3) C18A—C19A—H19A 119.9
C4B—C3B—H3BA 107.8 C21A—C20A—C19A 121.3 (3)
C2B—C3B—H3BA 107.8 C21A—C20A—H20A 119.3
C18B—C3B—H3BA 112.0 (3) C20A—C21A—C22A 118.1 (3)
C9B—C4B—C5B 121.0 (3) C20A—C21A—C24A 121.5 (3)
C9B—C4B—C3B 120.5 (3) C18A—C21A—C24A 120.3 (3)
C5B—C4B—C3B 118.4 (3) C22A—C21A—C24A 120.9 (3)
O1B—C5B—C4B 121.8 (3) C18A—C23A—C22A 120.9 (3)
O1B—C5B—C6B 118.3 (3) C21A—C22A—C23A 121.1 (3)
C4B—C5B—C6B 119.9 (3) C21A—C22A—H22A 119.4
C4B—C5B—C6B 119.9 (3) C23A—C22A—H22A 119.4
C16B—C6B—C7B 110.4 (4) C18A—C23A—C22A 120.9 (3)
C16B—C6B—C7B 111.1 (3) C18A—C23A—H23A 119.5
C7B—C6B—C5B 110.8 (3) C18A—C23A—H23A 119.5
C7B—C6B—C17B 107.6 (4) C25A—C24A—C29A 120.1 (5)
C7B—C6B—C17B 111.8 (3) C25A—C24A—C21A 121.5 (4)
C5B—C6B—C17B 105.0 (3) C25A—C24A—C21A 120.2 (4)
C6B—C7B—C8B 114.0 (3) C24A—C25A—C26A 120.6 (5)
C6B—C7B—C8B 114.0 (3) C24A—C25A—H25A 119.7
C8B—C7B—H7BA 108.8 C26A—C25A—H25A 119.7
C8B—C7B—H7BA 108.8 C27A—C26A—C25A 120.3 (5)
C6B—C7B—H7BB 108.8 C27A—C26A—H26A 119.9
C8B—C7B—H7BB 108.8 C27A—C26A—H26A 119.9
H7BA—C7B—H7BB 107.7 C25A—C26A—H26A 119.9
C9B—C8B—C7B 110.4 (3) C26A—C27A—C28A 119.8 (4)
C9B—C8B—H8BA 109.6 C26A—C27A—H27A 120.1
C7B—C8B—H8BA 109.6 C28A—C27A—H27A 120.1
C9B—C8B—H8BB 109.6 C27A—C28A—C29A 120.7 (5)
C7B—C8B—H8BB 109.6 C27A—C28A—H28A 119.7
H8BA—C8B—H8BB 108.1 C29A—C28A—H28A 119.7
C4B—C9B—N1B 120.5 (3) C28A—C29A—C24A 120.3 (5)
C4B—C9B—C8B 123.4 (3) C28A—C29A—H29A 119.9
N1B—C9B—C8B 116.0 (3) C24A—C29A—H29A 119.9
C1B—C10B—H10D 109.5

C9C—N1C—C1C—C2C −13.3 (5) C5B—C6B—C7B—C8B −49.0 (5)
C9C—N1C—C1C—C10C 165.7 (3) C17B—C6B—C7B—C8B 67.8 (5)
N1C—C1C—C2C—C11C 167.0 (3) C6B—C7B—C8B—C9B 48.9 (5)
C10C—C1C—C2C—C11C −11.9 (6) C5B—C4B—C9B—N1B 171.9 (3)
N1C—C1C—C2C—C3C −11.3 (5) C3B—C4B—C9B—N1B −6.1 (5)
C10C—C1C—C2C—C3C 169.8 (4) C5B—C4B—C9B—C8B 5.5 (5)
C1C—C2C—C3C—C18C −94.9 (4) C3B—C4B—C9B—C8B 176.5 (3)
C11C—C2C—C3C—C18C 86.6 (4) C1B—N1B—C9B—C4B −13.2 (5)
C1C—C2C—C3C—C4C 29.8 (4) C1B—N1B—C9B—C8B 164.3 (3)
C11C—C2C—C3C—C4C −148.6 (3) C7B—C8B—C9B—C4B −21.2 (5)
C18C—C3C—C4C—C9C 96.0 (4) C7B—C8B—C9B—N1B 161.3 (3)
C2C—C3C—C4C—C9C −27.9 (5) C12B—O3B—C11B—O2B −6.2 (6)
C18C—C3C—C4C—C5C −83.8 (7) C12B—O3B—C11B—C2B 172.5 (4)
C2C—C3C—C4C—C5C 152.3 (7) C1B—C2B—C11B—O2B 162.4 (4)
| Bond                        | Angle (°)        | Bond                        | Angle (°)        |
|-----------------------------|------------------|-----------------------------|------------------|
| C18C—C3C—C4C—C5F          | −76.5 (17)       | C3B—C2B—C11B—O2B          | −14.1 (5)        |
| C2C—C3C—C4C—C5F          | 159.6 (16)       | C1B—C2B—C11B—O3B          | −16.4 (6)        |
| C5C—C4C—C9C—N1C          | −172.9 (7)       | C3B—C2B—C11B—O3B          | 167.1 (3)        |
| C3C—C4C—C9C—N1C          | 7.3 (5)          | C11B—O3B—C12B—C15B        | 62.0 (6)         |
| C5F—C4C—C9C—N1C          | 179.1 (18)       | C11B—O3B—C12B—C13B        | −63.1 (5)        |
| C3C—C4C—C9C—C8F          | −173 (3)         | C11B—O3B—C12B—C14B        | −179.9 (4)       |
| C5F—C4C—C9C—C8F          | −1 (4)           | C4B—C3B—C18B—C23B         | 46.4 (4)         |
| C5C—C4C—C9C—C8C          | 6.9 (14)         | C2B—C3B—C18B—C23B         | −77.4 (4)        |
| C3C—C4C—C9C—C8C          | −172.9 (11)      | C4B—C3B—C18B—C19B         | −137.8 (3)       |
| C1C—N1C—C9C—C4C          | 15.4 (5)         | C2B—C3B—C18B—C19B         | 98.3 (4)         |
| C1C—N1C—C9C—C8F          | −164 (3)         | C23B—C18B—C19B—C20B       | 0.0 (5)          |
| C1C—N1C—C9C—C8C          | −164.4 (10)      | C3B—C18B—C19B—C20B        | −175.9 (3)       |
| C12C—O3C—C11C—O2C        | 3.1 (6)          | C18B—C19B—C20B—C21B       | 0.4 (6)          |
| C12C—O3C—C11C—C2C        | −174.1 (4)       | C19B—C20B—C21B—C22B       | −0.1 (6)         |
| C1C—C2C—C11C—O2C        | −175.7 (4)       | C19B—C20B—C21B—C24B       | 177.7 (4)        |
| C3C—C2C—C11C—O2C        | 2.7 (6)          | C20B—C21B—C22B—C23B       | −0.5 (6)         |
| C1C—C2C—C11C—O3C        | 1.6 (6)          | C24B—C21B—C22B—C23B       | −178.4 (4)       |
| C3C—C2C—C11C—O3C        | −180.0 (3)       | C19B—C18B—C23B—C22B       | −0.7 (6)         |
| C11C—O3C—C12C—C15C       | −66.1 (5)        | C3B—C18B—C23B—C22B        | 175.2 (3)        |
| C11C—O3C—C12C—C13C       | 58.8 (5)         | C21B—C22B—C23B—C18B       | 0.9 (6)          |
| C11C—O3C—C12C—C14C       | 176.2 (4)        | C20B—C21B—C24B—C29B       | 46.5 (6)         |
| C9C—C4C—C5C—O1C         | 176.3 (8)        | C22B—C21B—C24B—C29B       | −153.7 (4)       |
| C3C—C4C—C5C—O1C         | −3.9 (14)        | C20B—C21B—C24B—C25B       | −131.0 (5)       |
| C9C—C4C—C5C—C6C         | −15.8 (12)       | C22B—C21B—C24B—C25B       | 46.9 (6)         |
| C3C—C4C—C5C—C6C         | 164.0 (6)        | C29B—C24B—C25B—C26B       | −0.2 (8)         |
| O1C—C5C—C6C—C16C        | 87.0 (11)        | C21B—C24B—C25B—C26B       | 177.3 (5)        |
| C4C—C5C—C6C—C16C        | −81.2 (9)        | C24B—C25B—C26B—C27B       | −0.6 (9)         |
| O1C—C5C—C6C—C17C        | −32.3 (12)       | C25B—C26B—C27B—C28B       | 1.1 (9)          |
| C4C—C5C—C6C—C17C        | 159.4 (8)        | C26B—C27B—C28B—C29B       | −0.7 (8)         |
| O1C—C5C—C6C—C17C        | −152.3 (9)       | C25B—C24B—C29B—C28B       | 0.7 (7)          |
| C4C—C5C—C6C—C17C        | 39.5 (11)        | C21B—C24B—C29B—C28B       | −176.9 (4)       |
| C16C—C6C—C7C—C8C        | 62.9 (10)        | C27B—C28B—C29B—C24B       | −0.2 (7)         |
| C17C—C6C—C7C—C8C        | −175.6 (9)       | C9A—N1A—C1A—C2A           | −13.7 (5)        |
| C5C—C6C—C7C—C8C        | −56.1 (11)       | C9A—N1A—C1A—C10A          | 166.0 (3)        |
| C6C—C7C—C8C—C9C        | 47.6 (15)        | N1A—C1A—C2A—C11A          | 168.8 (3)        |
| C4C—C9C—C8C—C7C        | −22.9 (18)       | C10A—C1A—C2A—C11A         | −10.8 (6)        |
| N1C—C9C—C8C—C7C        | 156.9 (8)        | N1A—C1A—C2A—C3A           | −8.3 (5)         |
| C9C—C4C—C5F—O1C        | 165 (2)          | C10A—C1A—C2A—C3A          | 172.1 (3)        |
| C3C—C4C—C5F—O1C        | −23 (4)          | C1A—C2A—C3A—C4A           | 25.7 (4)         |
| C9C—C4C—C5F—C6F        | 12 (3)           | C1A—C2A—C3A—C4A           | 25.7 (4)         |
| C3C—C4C—C5F—C6F        | −175.9 (17)      | C1A—C2A—C3A—C18A          | −99.0 (4)        |
| O1C—C5F—C6F—C16F       | 50 (3)           | C11A—C2A—C3A—C18A         | 83.6 (4)         |
| C4C—C5F—C6F—C16F       | −156 (2)         | C2A—C3A—C4A—C9A           | −24.3 (4)        |
| O1C—C5F—C6F—C7F        | 169 (3)          | C18A—C3A—C4A—C9A          | 98.0 (4)         |
| C4C—C5F—C6F—C7F        | −37 (3)          | C2A—C3A—C4A—C5A           | 155.9 (3)        |
| O1C—C5F—C6F—C17F       | −67 (3)          | C18A—C3A—C4A—C5A          | −81.7 (4)        |
| C4C—C5F—C6F—C17F       | 86 (3)           | C9A—C4A—C5A—O1A           | 176.7 (3)        |
| C16F—C6F—C7F—C8F       | 170 (3)          | C3A—C4A—C5A—O1A           | −3.5 (5)         |
| Bond Type | Angle (°) | Bond Type | Angle (°) |
|-----------|-----------|-----------|-----------|
| C17F—C6F—C7F—C8F | -68 (3) | C9A—C4A—C5A—C6A | -4.4 (5) |
| C5F—C6F—C7F—C8F | 54 (3) | C3A—C4A—C5A—C6A | 175.4 (3) |
| C4C—C9C—C8F—C7F | 18 (6) | O1A—C5A—C6A—C17A | -33.9 (5) |
| N1C—C9C—C8F—C7F | -162 (3) | C4A—C5A—C6A—C17A | 147.2 (4) |
| C6F—C7F—C8F—C9C | -46 (5) | O1A—C5A—C6A—C7A | -154.9 (3) |
| C2C—C3C—C18C—C23C | 74.7 (4) | C4A—C5A—C6A—C7A | 26.2 (5) |
| C4C—C3C—C18C—C23C | -48.2 (4) | C4A—C5A—C6A—C7A | 67.6 (4) |
| C2C—C3C—C18C—C19C | -100.8 (4) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C4C—C3C—C18C—C19C | 136.3 (3) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C23C—C18C—C19C—C20C | -0.1 (5) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C3C—C18C—C19C—C20C | 175.6 (3) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C18C—C19C—C20C—C21C | -1.6 (6) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C19C—C20C—C21C—C22C | 1.7 (6) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C20C—C21C—C22C—C23C | -177.8 (4) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C22C—C21C—C22C—C23C | -0.2 (6) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C2C—C3C—C18C—C23C | 179.3 (4) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C24C—C21C—C22C—C23C | -1.5 (6) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C2C—C3C—C18C—C19C | 1.6 (5) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C4C—C3C—C18C—C19C | 174.1 (3) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C2C—C3C—C18C—C23C | 34.4 (6) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C22C—C21C—C24C—C25C | -145.0 (5) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C22C—C21C—C24C—C25C | -147.3 (4) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C2C—C3C—C18C—C22C | 33.3 (6) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C2C—C3C—C18C—C22C | -0.2 (9) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C29C—C24C—C25C—C26C | 178.1 (5) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C24C—C25C—C26C—C27C | -1.0 (10) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C25C—C26C—C27C—C28C | 1.5 (10) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C26C—C27C—C28C—C29C | -0.8 (9) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C27C—C28C—C29C—C30C | -0.5 (8) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C25C—C24C—C29C—C30C | 9.7 (7) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C21C—C24C—C29C—C30C | -177.4 (4) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C2B—C1B—N1B—C9B | 11.4 (5) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C10B—C1B—N1B—C9B | -167.1 (3) | C1A—N1A—C9A—C4A | 15.1 (5) |
| N1B—C1B—C2B—C11B | -166.7 (3) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C10B—C1B—C2B—C11B | 11.5 (6) | C1A—N1A—C9A—C4A | 15.1 (5) |
| N1B—C1B—C2B—C3B | 9.6 (5) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C10B—C1B—C2B—C3B | -172.2 (4) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C1B—C2B—C3B—C4B | -25.4 (4) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C11B—C2B—C3B—C4B | 151.2 (3) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C1B—C2B—C3B—C4B | 99.2 (4) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C11B—C2B—C3B—C4B | -84.1 (4) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C2B—C3B—C4B—C9B | 23.8 (4) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C18B—C3B—C4B—C9B | 100.0 (4) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C2B—C3B—C4B—C5B | -154.2 (3) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C18B—C3B—C4B—C5B | 82.0 (4) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C9B—C4B—C5B—O1B | -172.8 (3) | C1A—N1A—C9A—C4A | -165.3 (3) |
| C3B—C4B—C5B—O1B | 5.1 (5) | C1A—N1A—C9A—C4A | 15.1 (5) |
| C9B—C4B—C5B—C6B | 5.4 (5) | C1A—N1A—C9A—C4A | -165.3 (3) |

*Acta Cryst. (2022), E78, 798-803*
| Bond                  | Value (°)  |
|----------------------|------------|
| C3B—C4B—C5B—C6B    | −176.6 (3) |
| O1B—C5B—C6B—C16B   | −36.6 (5)  |
| C4B—C5B—C6B—C16B   | 145.1 (4)  |
| O1B—C5B—C6B—C7B    | −159.7 (3) |
| C4B—C5B—C6B—C7B    | 22.0 (5)   |
| O1B—C5B—C6B—C16B   | 79.4 (4)   |
| C4B—C5B—C6B—C7B    | −98.9 (4)  |
| C16B—C6B—C7B—C8B   | −172.5 (4) |

Hydrogen-bond geometry (Å, °)

Cg4, Cg8, Cg12 and Cg13 are the centroids of the C18C–C23C, C18A–C23A, C18B–C23B, and C18B–C29B rings, respectively.

| D—H···A     | D—H   | H···A | D···A   | D—H···A |
|-------------|-------|-------|---------|---------|
| N1C—H1NC···O1B | 0.92 (5) | 1.94 (5) | 2.843 (4) | 165 (5) |
| N1B—H1N4···O1A  | 0.95 (4) | 1.88 (4) | 2.811 (4) | 168 (3) |
| N1A—H1N4···O1A  | 0.93 (5) | 1.92 (5) | 2.842 (4) | 174 (4) |
| C3C—H3CA···O2C  | 1.00  | 2.41  | 2.793 (4) | 102    |
| C10A—H10B···O1A  | 0.98  | 2.60  | 3.443 (5) | 145    |
| C10B—H10F···O1C  | 0.98  | 2.47  | 3.302 (5) | 143    |
| C10C—H10G···O3C  | 0.98  | 2.31  | 2.704 (4) | 103    |
| C3A—H3BC···O2B   | 1.00  | 2.40  | 2.795 (4) | 103    |
| C13A—H13A···O2A  | 0.98  | 2.45  | 2.978 (7) | 113    |
| C13B—H13D···O2B  | 0.98  | 2.47  | 3.023 (6) | 115    |
| C13C—H13G···O2C  | 0.98  | 2.53  | 2.958 (7) | 106    |
| C15A—H15A···O2A  | 0.98  | 2.41  | 2.999 (7) | 118    |
| C15B—H15D···O2B  | 0.98  | 2.41  | 2.965 (6) | 116    |
| C15C—H15G···O2C  | 0.98  | 2.49  | 3.022 (5) | 114    |
| C3A—H3CA···O2A   | 1.00  | 2.42  | 2.812 (5) | 103    |
| C23A—H23A···O2A  | 0.95  | 2.57  | 3.403 (4) | 147    |
| C23B—H23B···O2C  | 0.95  | 2.55  | 3.389 (4) | 147    |
| C23C—H23C···O2B  | 0.95  | 2.60  | 3.407 (4) | 144    |
| C15A—H15B···Cg13 | 0.98  | 2.82  | 3.771 (6) | 165    |
| C27A—H27A···Cg4  | 0.95  | 2.75  | 3.578 (4) | 146    |
| C27B—H27B···Cg8  | 0.95  | 2.63  | 3.493 (5) | 150    |
| C27C—H27C···Cg12 | 0.95  | 2.84  | 3.632 (7) | 142    |

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