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# *N*-(1,3-Dioxo-2,3-dihydro-1*H*-isoindol-2-yl)-4,4″-difluoro-5′-hydroxy-1,1′:3′,1″-terphenyl-4′-carboxamide

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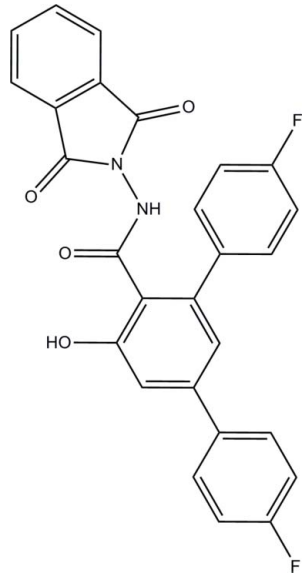
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; disorder in main residue; $R$ factor = 0.056; $wR$ factor = 0.168; data-to-parameter ratio = 22.3.

The asymmetric unit of the title compound, $C_{27}H_{16}F_2N_2O_4$, consists of two crystallographically independent molecules (*A* and *B*). In molecule *B*, the isoindoline-1,3-dione ring system is disordered over two set of sites with a site-occupancy ratio of 0.658 (12):0.342 (12). In molecule *A*, the fluoro-substituted benzene rings make dihedral angles of 18.36 (8) and 46.37 (8)° with the central benzene ring, whereas the corresponding angles are 40.90 (8) and 52.89 (9)° in molecule *B*. The isoindoline ring system in molecule *A* and the major and minor components of the disordered isoindoline ring system in molecule *B* make dihedral angles of 58.50 (4), 54.13 (16) and 70.01 (28) °, respectively, with their attached benzene rings, linked through the amide group. An intramolecular O—H···O hydrogen bond generates an *S*(6) ring in each molecule. In the crystal, molecules are linked by N—H···O, C—H···F and C—H···O hydrogen bonds into sheets lying parallel to the *bc* plane. The crystal studied was a non-merohedral twin with a refined twin component ratio of 0.9316 (8):0.0684 (8).

## Related literature

For related structures and background to terphenyls and their oxadiazole derivatives, see: Fun *et al.* (2012*a*,*b*); Samshuddin *et al.* (2011). For the planarity of isoindoline, see: Asad *et al.* (2011). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).




## Experimental

### Crystal data

$C_{27}H_{16}F_2N_2O_4$
$M_r$ = 470.42
Monoclinic, $P2_1/c$
$a$ = 24.8732 (10) Å
$b$ = 8.9875 (4) Å
$c$ = 21.3722 (9) Å
$\beta$ = 114.921 (1)°
$V$ = 4332.9 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 100 K
0.41 × 0.31 × 0.14 mm

### Data collection

Bruker APEX DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.956, $T_{max}$ = 0.985
16713 measured reflections
16713 independent reflections
12698 reflections with $I > 2\sigma(I)$

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.168
$S$ = 1.05
16713 reflections
748 parameters
45 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.63 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.90 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1*A*—H1*NA*···O2*A*$^{i}$ | 0.80 (3) | 2.02 (3) | 2.8000 (19) | 166 (3) |
| O1*B*—H1*OB*···O2*B* | 0.88 (3) | 1.79 (4) | 2.5663 (17) | 145 (4) |
| N1*B*—H1*NB*···O2*B*$^{ii}$ | 0.91 (3) | 2.04 (3) | 2.779 (2) | 138 (2) |
| O1*A*—H1*OA*···O2*A* | 0.82 (3) | 1.94 (3) | 2.6402 (18) | 143 (3) |
| C2*A*—H2*AA*···F2*A*$^{iii}$ | 0.93 | 2.45 | 3.160 (2) | 133 |
| C4*B*—H4*BA*···O3*B*$^{iv}$ | 0.93 | 2.41 | 3.271 (7) | 154 |
| C14*B*—H14*B*···O3*B*$^{v}$ | 0.93 | 2.44 | 3.293 (6) | 152 |
| C25*B*—H25*B*···O1*B*$^{vi}$ | 0.93 | 2.47 | 3.209 (3) | 136 |

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $-x, -y+2, -z$; (v) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (vi) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine

‡ Thomson Reuters ResearcherID: A-3561-2009.

structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6906).

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# supporting information

*Acta Cryst.* (2012). E**68**, o2619–o2620 [doi:10.1107/S160053681203365X]

## *N*-(1,3-Dioxo-2,3-dihydro-1*H*-isoindol-2-yl)-4,4′′-difluoro-5′-hydroxy-1,1′:3′,1′′-terphenyl-4′-carboxamide

**Hoong-Kun Fun, Tze Shyang Chia, S. Samshuddin, B. Narayana and B. K. Sarojini**

### S1. Comment

In continuation of our work on synthesis of various terphenyl derivatives (Fun *et al.*, 2012*a*,*b*), the title compound was prepared and its crystal structure is reported. The starting material of the title compound was prepared from 4,4′-difluoro chalcone by several steps (Samshuddin *et al.*, 2011).

The asymmetric unit of the title compound consists of two crystallographically independent molecules (*A* and *B*) as shown in Fig. 1. Each molecule contains one benzene ring [C7–C12], two fluoro-substituted benzene rings [C1–C6 & C13–C18] and an isoindoline-1,3-dione ring system [N2/O3/O4/C20–C27]. In molecule *B*, isoindoline-1,3-dione ring system is disordered over two positions with a site-occupancy ratio of 0.658 (12):0.342 (12). In molecule *A*, the fluoro-substituted benzene rings make dihedral angles of 18.36 (8) and 46.37 (8)° with the C7–C12 benzene ring, whereas the corresponding angles are 40.90 (8) and 52.89 (9)° in molecule *B*. The isoindoline ring systems [N2A/C20A–C27A, N2B/C20B–C27B & N2X/C20X–C27X; maximum deviations = 0.035 (1), 0.075 (4) and 0.084 (18) Å, respectively] make dihedral angles of 58.50 (4), 54.13 (16) and 70.01 (28) °, respectively with their attached C7–C12 benzene ring. An intramolecular O—H···O hydrogen bond (Table 1) generates an S(6) ring motif (Fig. 1; Bernstein *et al.*, 1995) in each molecule. The bond lengths and angles are comparable to those found in related structures (Fun *et al.*, 2012*a*,*b*)

In the crystal (Fig. 2), molecules are linked by N1A—H1NA···O2A, N1B—H1NB···O2B, C2A—H2AA···F2A, C4B—H4BA···O3B, C14B—H14B···O3B and C25B—H25B···O1B hydrogen bonds into sheets parallel to *bc* plane.

### S2. Experimental

A mixture of 4,4′′-difluoro-5′-hydroxy-1,1′:3′,1′′-terphenyl-4′-carbohydrazide (3.40 g, 0.01 mol) and phthalic anhydride (1.48 g, 0.01 mol) was dissolved in acetic acid (25 ml) and heated to reflux for 6 h. The reaction mixture was then poured into ice cold water, filtered and crystallized from ethanol. Colourless blocks were grown from DMF solution by slow evaporation method and yield of the compound was 76%. (m.p. 506 K).

### S3. Refinement

N-bound and O-bound H atoms were located in a difference fourier map and refined freely [N1A—H1NA = 0.80 (3) Å, N1B—H1NB = 0.91 (3) Å, O1A—H1OA = 0.82 (3) Å, O1B—H1OB = 0.88 (3) Å]. The remaining H atoms were positioned geometrically [C—H = 0.93 Å] and refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C). FLAT restraint was applied to the N2/O3/O4/C20–C27 ring system in molecule *A* and minor component of molecule *B* so that the planarity of isoindoline ring is agreed with that found in a related structure (Asad *et al.*, 2011). Ten outliers, (0 2 3), (1 0 0), ($\overline{3}$ 3 5), ($\overline{20}$ 0 6), (12 0 6), ($\overline{21}$ 3 6), (10 1 7), ($\overline{15}$ 6 6), (7 4 6) and ($\overline{14}$ 5 6), were omitted in the final refinement. The crystal studied was a non-merohedral twin with BASF = 0.0684 (8).

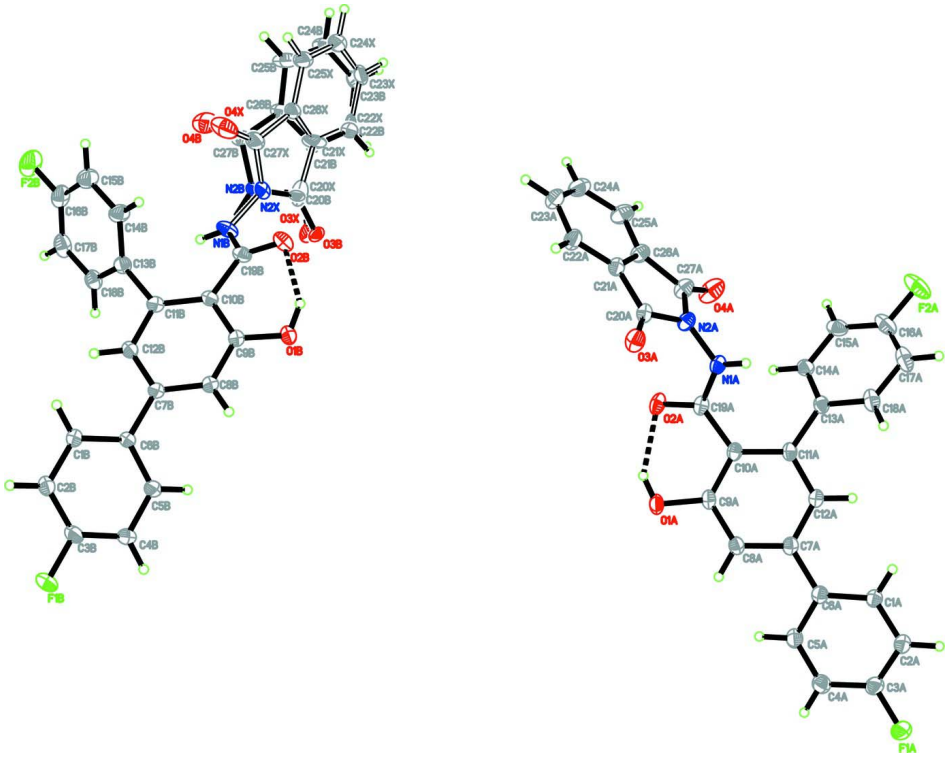


**Figure 1**

The molecular structure of the title compound with 50% probability displacement ellipsoids. Intramolecular hydrogen bonds are shown by dashed lines.

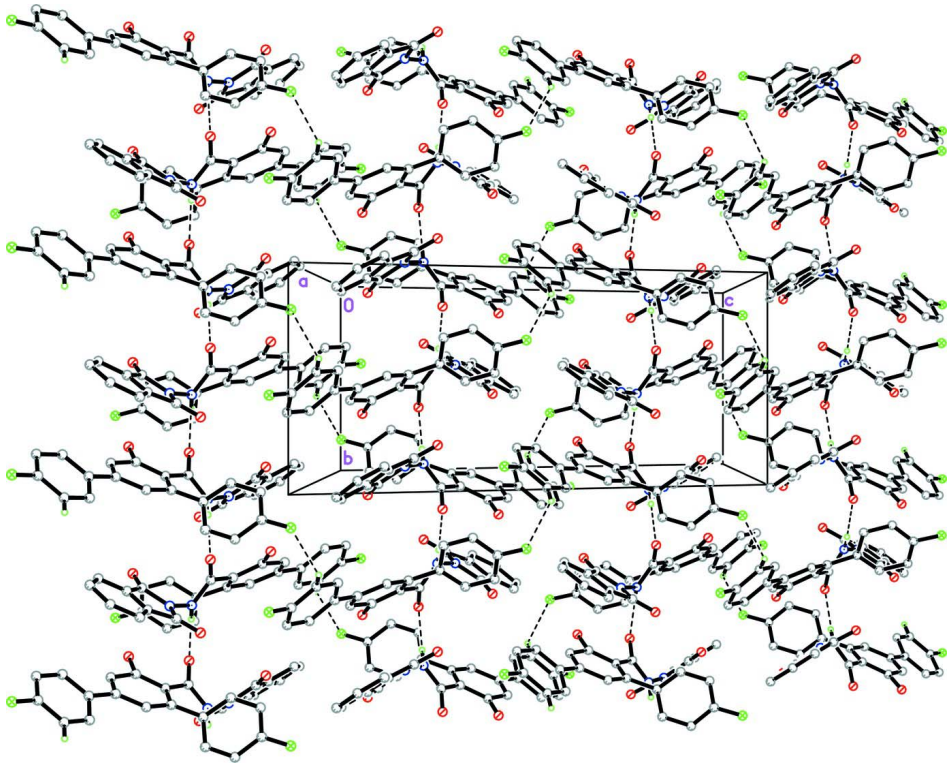


**Figure 2**

The crystal packing of the title compound. The dashed lines represent the hydrogen bonds.

**_N_-(1,3-Dioxo-2,3-dihydro-1_H_-isoindol-2-yl)-4,4′′-difluoro- 5′-hydroxy-1,1′:3′,1′′-terphenyl-4′-carboxamide**

*Crystal data*

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$M_r = 470.42$
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$c = 21.3722$ (9) Å
$\beta = 114.921$ (1)°
$V = 4332.9$ (3) Å$^3$
$Z = 8$
$F(000) = 1936$
$D_x = 1.442$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9881 reflections
$\theta = 2.8$–$33.2°$
$\mu = 0.11$ mm$^{-1}$
$T = 100$ K
Block, colourless
0.41 × 0.31 × 0.14 mm

*Data collection*

Bruker APEX DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.956$, $T_{max} = 0.985$
16713 measured reflections
16713 independent reflections
12698 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 33.3°$, $\theta_{min} = 0.9°$
$h = -38 \rightarrow 34$
$k = -13 \rightarrow 13$
$l = 0 \rightarrow 32$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.168$
$S = 1.05$
16713 reflections
748 parameters
45 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
$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2 + 2.8746P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.63$ e Å$^{-3}$
$\Delta\rho_{min} = -0.90$ e Å$^{-3}$

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| F1A | 0.70185 (5) | 0.57672 (16) | −0.07644 (6) | 0.0364 (3) | |
| F2A | 0.74047 (5) | 0.31572 (16) | 0.47234 (7) | 0.0448 (3) | |
| O1A | 0.44381 (5) | 0.67527 (14) | 0.09291 (6) | 0.0239 (2) | |
| O2A | 0.45373 (5) | 0.64374 (13) | 0.22015 (7) | 0.0244 (2) | |
| O3A | 0.37372 (5) | 0.32205 (15) | 0.22722 (7) | 0.0272 (2) | |
| O4A | 0.52736 (6) | 0.57608 (18) | 0.39267 (8) | 0.0384 (3) | |
| N1A | 0.49213 (6) | 0.42265 (15) | 0.26521 (7) | 0.0194 (2) | |
| N2A | 0.46069 (6) | 0.43104 (14) | 0.30464 (7) | 0.0200 (2) | |
| C1A | 0.66264 (7) | 0.46269 (19) | 0.06103 (8) | 0.0220 (3) | |
| H1AA | 0.6752 | 0.3957 | 0.0976 | 0.026* | |
| C2A | 0.69280 (7) | 0.4694 (2) | 0.01934 (9) | 0.0255 (3) | |
| H2AA | 0.7255 | 0.4091 | 0.0278 | 0.031* | |
| C3A | 0.67274 (7) | 0.5687 (2) | −0.03518 (9) | 0.0258 (3) | |
| C4A | 0.62450 (7) | 0.6598 (2) | −0.04955 (9) | 0.0262 (3) | |
| H4AA | 0.6116 | 0.7240 | −0.0872 | 0.031* | |
| C5A | 0.59568 (7) | 0.65329 (19) | −0.00633 (9) | 0.0233 (3) | |
| H5AA | 0.5637 | 0.7160 | −0.0146 | 0.028* | |
| C6A | 0.61381 (7) | 0.55424 (17) | 0.04938 (8) | 0.0193 (3) | |
| C7A | 0.58244 (6) | 0.54752 (17) | 0.09474 (8) | 0.0185 (2) | |
| C8A | 0.52569 (6) | 0.60577 (17) | 0.07381 (8) | 0.0194 (3) | |
| H8AA | 0.5062 | 0.6442 | 0.0295 | 0.023* | |
| C9A | 0.49761 (6) | 0.60762 (17) | 0.11803 (8) | 0.0187 (3) | |

| | | | | |
|---|---|---|---|---|
| C10A | 0.52419 (6) | 0.54063 (16) | 0.18387 (8) | 0.0177 (2) |
| C11A | 0.58238 (6) | 0.48200 (16) | 0.20595 (8) | 0.0177 (2) |
| C12A | 0.61013 (6) | 0.48774 (17) | 0.16141 (8) | 0.0186 (3) |
| H12A | 0.6484 | 0.4506 | 0.1764 | 0.022* |
| C13A | 0.61965 (6) | 0.42961 (17) | 0.27708 (8) | 0.0190 (3) |
| C14A | 0.62408 (7) | 0.51251 (19) | 0.33414 (8) | 0.0215 (3) |
| H14A | 0.5999 | 0.5952 | 0.3279 | 0.026* |
| C15A | 0.66434 (7) | 0.4728 (2) | 0.40044 (9) | 0.0270 (3) |
| H15A | 0.6673 | 0.5278 | 0.4386 | 0.032* |
| C16A | 0.69952 (8) | 0.3503 (2) | 0.40793 (10) | 0.0319 (4) |
| C17A | 0.69626 (8) | 0.2637 (2) | 0.35338 (11) | 0.0319 (4) |
| H17A | 0.7204 | 0.1806 | 0.3604 | 0.038* |
| C18A | 0.65589 (7) | 0.30408 (19) | 0.28748 (10) | 0.0254 (3) |
| H18A | 0.6529 | 0.2471 | 0.2498 | 0.030* |
| C19A | 0.48859 (6) | 0.54052 (16) | 0.22477 (8) | 0.0188 (3) |
| C20A | 0.40094 (6) | 0.38583 (17) | 0.28064 (8) | 0.0192 (3) |
| C21A | 0.38250 (7) | 0.43651 (17) | 0.33479 (8) | 0.0199 (3) |
| C22A | 0.32915 (7) | 0.4177 (2) | 0.33958 (9) | 0.0266 (3) |
| H22A | 0.2982 | 0.3641 | 0.3066 | 0.032* |
| C23A | 0.32378 (8) | 0.4828 (2) | 0.39620 (10) | 0.0297 (3) |
| H23A | 0.2885 | 0.4722 | 0.4009 | 0.036* |
| C24A | 0.36994 (9) | 0.5627 (2) | 0.44533 (10) | 0.0308 (4) |
| H24A | 0.3649 | 0.6058 | 0.4820 | 0.037* |
| C25A | 0.42400 (9) | 0.5795 (2) | 0.44060 (10) | 0.0305 (4) |
| H25A | 0.4553 | 0.6315 | 0.4739 | 0.037* |
| C26A | 0.42891 (7) | 0.51557 (19) | 0.38443 (9) | 0.0228 (3) |
| C27A | 0.47978 (7) | 0.51708 (19) | 0.36511 (9) | 0.0243 (3) |
| F1B | −0.24301 (5) | 0.91133 (16) | −0.29187 (5) | 0.0347 (3) |
| F2B | −0.22044 (6) | 1.19023 (17) | 0.26237 (7) | 0.0440 (3) |
| O1B | 0.02966 (5) | 0.75887 (17) | 0.11463 (6) | 0.0279 (3) |
| O2B | 0.03502 (6) | 0.78615 (14) | 0.23665 (6) | 0.0256 (2) |
| N1B | −0.00874 (7) | 0.98785 (17) | 0.25626 (7) | 0.0249 (3) |
| C1B | −0.20753 (7) | 0.87878 (19) | −0.11017 (8) | 0.0210 (3) |
| H1BA | −0.2263 | 0.8584 | −0.0816 | 0.025* |
| C2B | −0.24027 (7) | 0.8785 (2) | −0.18146 (8) | 0.0239 (3) |
| H2BA | −0.2806 | 0.8575 | −0.2010 | 0.029* |
| C3B | −0.21122 (7) | 0.9102 (2) | −0.22228 (8) | 0.0242 (3) |
| C4B | −0.15137 (7) | 0.9400 (2) | −0.19595 (8) | 0.0270 (3) |
| H4BA | −0.1331 | 0.9604 | −0.2250 | 0.032* |
| C5B | −0.11913 (7) | 0.9385 (2) | −0.12468 (8) | 0.0245 (3) |
| H5BA | −0.0786 | 0.9572 | −0.1058 | 0.029* |
| C6B | −0.14672 (6) | 0.90931 (18) | −0.08102 (7) | 0.0189 (3) |
| C7B | −0.11148 (6) | 0.90581 (18) | −0.00535 (7) | 0.0192 (3) |
| C8B | −0.05588 (7) | 0.8402 (2) | 0.02207 (8) | 0.0222 (3) |
| H8BA | −0.0403 | 0.8024 | −0.0073 | 0.027* |
| C9B | −0.02312 (6) | 0.83030 (19) | 0.09311 (8) | 0.0204 (3) |
| C10B | −0.04459 (7) | 0.89221 (17) | 0.13910 (7) | 0.0180 (2) |
| C11B | −0.10190 (7) | 0.95784 (17) | 0.11118 (7) | 0.0184 (2) |

| | | | | | |
|---|---|---|---|---|---|
| C12B | −0.13399 (7) | 0.96299 (18) | 0.03979 (8) | 0.0196 (3) | |
| H12B | −0.1715 | 1.0057 | 0.0215 | 0.023* | |
| C13B | −0.13197 (7) | 1.01929 (18) | 0.15303 (8) | 0.0204 (3) | |
| C14B | −0.13921 (8) | 0.9340 (2) | 0.20379 (9) | 0.0255 (3) | |
| H14B | −0.1241 | 0.8378 | 0.2128 | 0.031* | |
| C15B | −0.16887 (9) | 0.9922 (2) | 0.24094 (10) | 0.0309 (4) | |
| H15B | −0.1736 | 0.9359 | 0.2748 | 0.037* | |
| C16B | −0.19113 (8) | 1.1348 (2) | 0.22641 (10) | 0.0306 (4) | |
| C17B | −0.18557 (8) | 1.2222 (2) | 0.17653 (9) | 0.0289 (3) | |
| H17B | −0.2012 | 1.3179 | 0.1677 | 0.035* | |
| C18B | −0.15578 (7) | 1.16279 (19) | 0.13971 (9) | 0.0237 (3) | |
| H18B | −0.1517 | 1.2197 | 0.1056 | 0.028* | |
| C19B | −0.00406 (7) | 0.88355 (17) | 0.21341 (8) | 0.0202 (3) | |
| O3B | 0.1114 (3) | 1.0874 (6) | 0.3230 (3) | 0.0205 (7) | 0.658 (12) |
| O4B | −0.03851 (17) | 0.8627 (7) | 0.36124 (16) | 0.0433 (10) | 0.658 (12) |
| N2B | 0.0251 (2) | 0.9875 (5) | 0.3257 (2) | 0.0126 (6) | 0.658 (12) |
| C20B | 0.0845 (3) | 1.0357 (9) | 0.3540 (2) | 0.0160 (14) | 0.658 (12) |
| C21B | 0.1069 (2) | 1.0054 (8) | 0.4280 (3) | 0.0175 (13) | 0.658 (12) |
| C22B | 0.1588 (4) | 1.0456 (16) | 0.4820 (4) | 0.0235 (17) | 0.658 (12) |
| H22B | 0.1884 | 1.0945 | 0.4742 | 0.028* | 0.658 (12) |
| C23B | 0.1665 (3) | 1.0115 (9) | 0.5491 (4) | 0.0254 (13) | 0.658 (12) |
| H23B | 0.2018 | 1.0369 | 0.5862 | 0.031* | 0.658 (12) |
| C24B | 0.1228 (2) | 0.9414 (8) | 0.56112 (18) | 0.0370 (11) | 0.658 (12) |
| H24B | 0.1293 | 0.9180 | 0.6061 | 0.044* | 0.658 (12) |
| C25B | 0.0686 (2) | 0.9044 (8) | 0.50666 (16) | 0.0413 (14) | 0.658 (12) |
| H25B | 0.0388 | 0.8569 | 0.5146 | 0.050* | 0.658 (12) |
| C26B | 0.0612 (2) | 0.9412 (6) | 0.44076 (18) | 0.0250 (8) | 0.658 (12) |
| C27B | 0.00860 (19) | 0.9190 (6) | 0.37426 (18) | 0.0258 (8) | 0.658 (12) |
| O3X | 0.1052 (6) | 1.1164 (11) | 0.3266 (7) | 0.0297 (19) | 0.342 (12) |
| O4X | −0.0235 (4) | 0.7929 (13) | 0.3521 (4) | 0.046 (3) | 0.342 (12) |
| N2X | 0.0342 (4) | 0.9593 (9) | 0.3252 (5) | 0.0195 (16) | 0.342 (12) |
| C20X | 0.0880 (7) | 1.0363 (19) | 0.3594 (6) | 0.029 (4) | 0.342 (12) |
| C21X | 0.1074 (6) | 1.0017 (19) | 0.4334 (6) | 0.031 (4) | 0.342 (12) |
| C22X | 0.1601 (7) | 1.041 (2) | 0.4886 (8) | 0.022 (3) | 0.342 (12) |
| H22C | 0.1870 | 1.1065 | 0.4838 | 0.026* | 0.342 (12) |
| C23X | 0.1700 (6) | 0.9752 (17) | 0.5524 (8) | 0.029 (3) | 0.342 (12) |
| H23C | 0.2036 | 1.0011 | 0.5916 | 0.034* | 0.342 (12) |
| C24X | 0.1306 (3) | 0.8728 (15) | 0.5579 (4) | 0.0333 (18) | 0.342 (12) |
| H24C | 0.1378 | 0.8349 | 0.6012 | 0.040* | 0.342 (12) |
| C25X | 0.0804 (3) | 0.8241 (14) | 0.5006 (3) | 0.035 (2) | 0.342 (12) |
| H25C | 0.0552 | 0.7520 | 0.5044 | 0.042* | 0.342 (12) |
| C26X | 0.0705 (3) | 0.8894 (11) | 0.4379 (3) | 0.0227 (14) | 0.342 (12) |
| C27X | 0.0197 (3) | 0.8682 (12) | 0.3690 (4) | 0.0273 (16) | 0.342 (12) |
| H1NA | 0.5124 (11) | 0.351 (3) | 0.2695 (12) | 0.025 (5)* | |
| H1OB | 0.0450 (15) | 0.749 (4) | 0.1599 (18) | 0.056 (9)* | |
| H1NB | −0.0342 (13) | 1.066 (3) | 0.2407 (14) | 0.039 (7)* | |
| H1OA | 0.4311 (13) | 0.675 (3) | 0.1226 (16) | 0.045 (8)* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1A | 0.0258 (5) | 0.0597 (8) | 0.0288 (5) | 0.0058 (5) | 0.0165 (4) | 0.0077 (5) |
| F2A | 0.0285 (6) | 0.0497 (8) | 0.0364 (6) | −0.0065 (5) | −0.0057 (5) | 0.0214 (6) |
| O1A | 0.0166 (5) | 0.0276 (6) | 0.0250 (5) | 0.0069 (4) | 0.0063 (4) | −0.0011 (4) |
| O2A | 0.0227 (5) | 0.0169 (5) | 0.0397 (7) | 0.0032 (4) | 0.0190 (5) | 0.0006 (5) |
| O3A | 0.0209 (5) | 0.0303 (6) | 0.0285 (6) | −0.0039 (5) | 0.0086 (4) | −0.0093 (5) |
| O4A | 0.0297 (6) | 0.0501 (9) | 0.0396 (7) | −0.0206 (6) | 0.0186 (6) | −0.0213 (7) |
| N1A | 0.0193 (5) | 0.0159 (5) | 0.0262 (6) | 0.0013 (4) | 0.0126 (5) | −0.0009 (5) |
| N2A | 0.0183 (5) | 0.0200 (6) | 0.0237 (6) | −0.0035 (4) | 0.0109 (5) | −0.0040 (5) |
| C1A | 0.0204 (6) | 0.0252 (7) | 0.0201 (6) | 0.0039 (5) | 0.0082 (5) | −0.0006 (5) |
| C2A | 0.0200 (6) | 0.0328 (8) | 0.0239 (7) | 0.0049 (6) | 0.0096 (6) | −0.0002 (6) |
| C3A | 0.0198 (6) | 0.0364 (9) | 0.0222 (7) | −0.0011 (6) | 0.0098 (5) | −0.0009 (6) |
| C4A | 0.0219 (7) | 0.0303 (8) | 0.0262 (7) | 0.0007 (6) | 0.0101 (6) | 0.0050 (6) |
| C5A | 0.0204 (6) | 0.0226 (7) | 0.0273 (7) | 0.0022 (5) | 0.0103 (6) | 0.0030 (6) |
| C6A | 0.0174 (6) | 0.0196 (6) | 0.0196 (6) | −0.0004 (5) | 0.0064 (5) | −0.0029 (5) |
| C7A | 0.0173 (6) | 0.0168 (6) | 0.0202 (6) | −0.0002 (5) | 0.0067 (5) | −0.0034 (5) |
| C8A | 0.0167 (6) | 0.0195 (6) | 0.0192 (6) | 0.0018 (5) | 0.0047 (5) | −0.0018 (5) |
| C9A | 0.0142 (5) | 0.0171 (6) | 0.0222 (6) | 0.0019 (5) | 0.0050 (5) | −0.0028 (5) |
| C10A | 0.0157 (5) | 0.0151 (6) | 0.0223 (6) | 0.0001 (4) | 0.0081 (5) | −0.0022 (5) |
| C11A | 0.0151 (5) | 0.0149 (6) | 0.0220 (6) | 0.0004 (4) | 0.0069 (5) | −0.0010 (5) |
| C12A | 0.0158 (5) | 0.0179 (6) | 0.0218 (6) | 0.0014 (5) | 0.0077 (5) | −0.0010 (5) |
| C13A | 0.0151 (5) | 0.0180 (6) | 0.0231 (6) | −0.0002 (5) | 0.0072 (5) | 0.0032 (5) |
| C14A | 0.0196 (6) | 0.0235 (7) | 0.0218 (7) | −0.0008 (5) | 0.0092 (5) | 0.0039 (5) |
| C15A | 0.0230 (7) | 0.0343 (9) | 0.0218 (7) | −0.0068 (6) | 0.0076 (6) | 0.0059 (6) |
| C16A | 0.0202 (7) | 0.0359 (9) | 0.0303 (8) | −0.0048 (6) | 0.0015 (6) | 0.0153 (7) |
| C17A | 0.0199 (7) | 0.0245 (8) | 0.0441 (10) | 0.0032 (6) | 0.0064 (7) | 0.0115 (7) |
| C18A | 0.0190 (6) | 0.0201 (7) | 0.0350 (8) | 0.0013 (5) | 0.0094 (6) | 0.0042 (6) |
| C19A | 0.0162 (6) | 0.0151 (6) | 0.0252 (7) | −0.0017 (5) | 0.0088 (5) | −0.0030 (5) |
| C20A | 0.0164 (6) | 0.0167 (6) | 0.0248 (7) | 0.0002 (5) | 0.0089 (5) | −0.0003 (5) |
| C21A | 0.0180 (6) | 0.0190 (6) | 0.0237 (7) | 0.0007 (5) | 0.0098 (5) | 0.0008 (5) |
| C22A | 0.0200 (7) | 0.0314 (8) | 0.0302 (8) | −0.0005 (6) | 0.0123 (6) | −0.0010 (6) |
| C23A | 0.0275 (8) | 0.0342 (9) | 0.0346 (9) | 0.0036 (7) | 0.0201 (7) | 0.0032 (7) |
| C24A | 0.0391 (9) | 0.0312 (9) | 0.0304 (8) | 0.0017 (7) | 0.0228 (8) | 0.0001 (7) |
| C25A | 0.0365 (9) | 0.0321 (9) | 0.0282 (8) | −0.0073 (7) | 0.0187 (7) | −0.0083 (7) |
| C26A | 0.0239 (7) | 0.0223 (7) | 0.0247 (7) | −0.0032 (5) | 0.0126 (6) | −0.0029 (6) |
| C27A | 0.0226 (7) | 0.0252 (7) | 0.0271 (7) | −0.0067 (6) | 0.0125 (6) | −0.0067 (6) |
| F1B | 0.0284 (5) | 0.0549 (8) | 0.0146 (4) | 0.0039 (5) | 0.0031 (4) | 0.0014 (4) |
| F2B | 0.0402 (7) | 0.0562 (8) | 0.0434 (7) | 0.0062 (6) | 0.0253 (6) | −0.0177 (6) |
| O1B | 0.0192 (5) | 0.0426 (7) | 0.0199 (5) | 0.0090 (5) | 0.0064 (4) | 0.0035 (5) |
| O2B | 0.0266 (6) | 0.0232 (6) | 0.0206 (5) | 0.0025 (4) | 0.0038 (4) | 0.0028 (4) |
| N1B | 0.0320 (7) | 0.0231 (6) | 0.0139 (5) | 0.0007 (5) | 0.0042 (5) | 0.0005 (5) |
| C1B | 0.0167 (6) | 0.0271 (7) | 0.0197 (6) | 0.0020 (5) | 0.0083 (5) | 0.0008 (5) |
| C2B | 0.0173 (6) | 0.0309 (8) | 0.0207 (7) | 0.0023 (6) | 0.0052 (5) | −0.0005 (6) |
| C3B | 0.0227 (7) | 0.0315 (8) | 0.0144 (6) | 0.0039 (6) | 0.0040 (5) | 0.0004 (6) |
| C4B | 0.0224 (7) | 0.0413 (10) | 0.0175 (6) | −0.0001 (6) | 0.0085 (5) | 0.0048 (6) |
| C5B | 0.0181 (6) | 0.0369 (9) | 0.0172 (6) | −0.0024 (6) | 0.0062 (5) | 0.0034 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6B | 0.0174 (6) | 0.0234 (7) | 0.0153 (6) | 0.0023 (5) | 0.0063 (5) | 0.0016 (5) |
| C7B | 0.0173 (6) | 0.0239 (7) | 0.0160 (6) | 0.0000 (5) | 0.0067 (5) | 0.0017 (5) |
| C8B | 0.0185 (6) | 0.0313 (8) | 0.0176 (6) | 0.0021 (6) | 0.0083 (5) | 0.0015 (6) |
| C9B | 0.0166 (6) | 0.0258 (7) | 0.0183 (6) | 0.0010 (5) | 0.0069 (5) | 0.0019 (5) |
| C10B | 0.0194 (6) | 0.0184 (6) | 0.0152 (6) | −0.0010 (5) | 0.0061 (5) | 0.0009 (5) |
| C11B | 0.0207 (6) | 0.0174 (6) | 0.0172 (6) | 0.0004 (5) | 0.0081 (5) | 0.0002 (5) |
| C12B | 0.0182 (6) | 0.0222 (7) | 0.0173 (6) | 0.0017 (5) | 0.0066 (5) | 0.0003 (5) |
| C13B | 0.0216 (6) | 0.0215 (7) | 0.0176 (6) | 0.0007 (5) | 0.0078 (5) | −0.0032 (5) |
| C14B | 0.0318 (8) | 0.0251 (7) | 0.0233 (7) | 0.0023 (6) | 0.0152 (6) | −0.0019 (6) |
| C15B | 0.0342 (9) | 0.0371 (9) | 0.0256 (8) | 0.0010 (7) | 0.0168 (7) | −0.0050 (7) |
| C16B | 0.0249 (7) | 0.0402 (10) | 0.0276 (8) | 0.0019 (7) | 0.0120 (6) | −0.0136 (7) |
| C17B | 0.0236 (7) | 0.0280 (8) | 0.0296 (8) | 0.0054 (6) | 0.0057 (6) | −0.0087 (6) |
| C18B | 0.0214 (6) | 0.0227 (7) | 0.0227 (7) | 0.0015 (5) | 0.0052 (5) | −0.0030 (6) |
| C19B | 0.0224 (6) | 0.0187 (6) | 0.0166 (6) | −0.0033 (5) | 0.0055 (5) | 0.0023 (5) |
| O3B | 0.0236 (14) | 0.0203 (19) | 0.0250 (11) | 0.0081 (13) | 0.0175 (10) | 0.0056 (12) |
| O4B | 0.0345 (14) | 0.061 (3) | 0.0298 (12) | −0.0243 (16) | 0.0094 (10) | 0.0012 (14) |
| N2B | 0.0137 (13) | 0.0123 (14) | 0.0111 (9) | 0.0031 (11) | 0.0045 (9) | 0.0000 (10) |
| C20B | 0.022 (2) | 0.019 (3) | 0.0083 (13) | 0.0040 (17) | 0.0074 (12) | 0.0013 (13) |
| C21B | 0.0114 (16) | 0.024 (3) | 0.017 (2) | −0.0079 (15) | 0.0058 (14) | −0.0025 (16) |
| C22B | 0.025 (3) | 0.027 (3) | 0.019 (2) | 0.004 (2) | 0.0098 (19) | 0.0037 (18) |
| C23B | 0.020 (2) | 0.030 (3) | 0.0182 (16) | 0.000 (2) | 0.0001 (13) | 0.0004 (17) |
| C24B | 0.0369 (19) | 0.052 (3) | 0.0166 (12) | −0.0129 (19) | 0.0060 (12) | 0.0039 (16) |
| C25B | 0.0365 (19) | 0.066 (3) | 0.0178 (12) | −0.027 (2) | 0.0075 (11) | 0.0057 (15) |
| C26B | 0.0249 (16) | 0.031 (2) | 0.0163 (11) | −0.0068 (14) | 0.0062 (10) | 0.0033 (13) |
| C27B | 0.0251 (15) | 0.033 (2) | 0.0170 (11) | −0.0101 (14) | 0.0070 (10) | 0.0006 (13) |
| O3X | 0.036 (3) | 0.016 (3) | 0.049 (4) | 0.014 (2) | 0.029 (2) | 0.010 (3) |
| O4X | 0.034 (3) | 0.057 (5) | 0.029 (3) | −0.028 (3) | −0.005 (2) | 0.015 (3) |
| N2X | 0.023 (3) | 0.018 (3) | 0.018 (2) | 0.012 (2) | 0.009 (2) | −0.001 (2) |
| C20X | 0.022 (5) | 0.012 (5) | 0.055 (8) | −0.005 (4) | 0.017 (5) | −0.006 (5) |
| C21X | 0.052 (7) | 0.034 (7) | 0.012 (4) | 0.009 (5) | 0.017 (4) | 0.001 (3) |
| C22X | 0.008 (4) | 0.022 (6) | 0.029 (5) | −0.002 (3) | 0.001 (3) | −0.011 (4) |
| C23X | 0.020 (3) | 0.041 (8) | 0.021 (3) | 0.013 (4) | 0.005 (2) | 0.002 (4) |
| C24X | 0.023 (2) | 0.053 (5) | 0.021 (3) | 0.000 (3) | 0.0058 (19) | 0.008 (3) |
| C25X | 0.022 (2) | 0.057 (6) | 0.024 (3) | −0.006 (3) | 0.0072 (19) | 0.013 (3) |
| C26X | 0.016 (2) | 0.029 (4) | 0.020 (2) | −0.003 (2) | 0.0045 (17) | 0.006 (2) |
| C27X | 0.022 (3) | 0.033 (4) | 0.022 (3) | −0.004 (3) | 0.005 (2) | 0.004 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F1A—C3A | 1.3585 (19) | C1B—C2B | 1.392 (2) |
| F2A—C16A | 1.359 (2) | C1B—C6B | 1.399 (2) |
| O1A—C9A | 1.3577 (18) | C1B—H1BA | 0.9300 |
| O1A—H1OA | 0.82 (3) | C2B—C3B | 1.377 (2) |
| O2A—C19A | 1.2449 (18) | C2B—H2BA | 0.9300 |
| O3A—C20A | 1.200 (2) | C3B—C4B | 1.378 (2) |
| O4A—C27A | 1.200 (2) | C4B—C5B | 1.391 (2) |
| N1A—C19A | 1.346 (2) | C4B—H4BA | 0.9300 |
| N1A—N2A | 1.3723 (18) | C5B—C6B | 1.396 (2) |

| | | | |
|---|---|---|---|
| N1A—H1NA | 0.80 (3) | C5B—H5BA | 0.9300 |
| N2A—C27A | 1.406 (2) | C6B—C7B | 1.480 (2) |
| N2A—C20A | 1.4123 (19) | C7B—C8B | 1.386 (2) |
| C1A—C2A | 1.387 (2) | C7B—C12B | 1.401 (2) |
| C1A—C6A | 1.400 (2) | C8B—C9B | 1.391 (2) |
| C1A—H1AA | 0.9300 | C8B—H8BA | 0.9300 |
| C2A—C3A | 1.383 (3) | C9B—C10B | 1.415 (2) |
| C2A—H2AA | 0.9300 | C10B—C11B | 1.421 (2) |
| C3A—C4A | 1.376 (2) | C10B—C19B | 1.482 (2) |
| C4A—C5A | 1.389 (2) | C11B—C12B | 1.393 (2) |
| C4A—H4AA | 0.9300 | C11B—C13B | 1.493 (2) |
| C5A—C6A | 1.400 (2) | C12B—H12B | 0.9300 |
| C5A—H5AA | 0.9300 | C13B—C18B | 1.398 (2) |
| C6A—C7A | 1.480 (2) | C13B—C14B | 1.400 (2) |
| C7A—C8A | 1.391 (2) | C14B—C15B | 1.393 (2) |
| C7A—C12A | 1.402 (2) | C14B—H14B | 0.9300 |
| C8A—C9A | 1.392 (2) | C15B—C16B | 1.379 (3) |
| C8A—H8AA | 0.9300 | C15B—H15B | 0.9300 |
| C9A—C10A | 1.413 (2) | C16B—C17B | 1.377 (3) |
| C10A—C11A | 1.421 (2) | C17B—C18B | 1.394 (2) |
| C10A—C19A | 1.484 (2) | C17B—H17B | 0.9300 |
| C11A—C12A | 1.392 (2) | C18B—H18B | 0.9300 |
| C11A—C13A | 1.485 (2) | O3B—C20B | 1.214 (5) |
| C12A—H12A | 0.9300 | O4B—C27B | 1.197 (4) |
| C13A—C14A | 1.393 (2) | N2B—C27B | 1.408 (5) |
| C13A—C18A | 1.402 (2) | N2B—C20B | 1.410 (6) |
| C14A—C15A | 1.394 (2) | C20B—C21B | 1.463 (6) |
| C14A—H14A | 0.9300 | C21B—C22B | 1.369 (7) |
| C15A—C16A | 1.373 (3) | C21B—C26B | 1.401 (5) |
| C15A—H15A | 0.9300 | C22B—C23B | 1.400 (8) |
| C16A—C17A | 1.375 (3) | C22B—H22B | 0.9300 |
| C17A—C18A | 1.390 (3) | C23B—C24B | 1.370 (7) |
| C17A—H17A | 0.9300 | C23B—H23B | 0.9300 |
| C18A—H18A | 0.9300 | C24B—C25B | 1.401 (5) |
| C20A—C21A | 1.485 (2) | C24B—H24B | 0.9300 |
| C21A—C22A | 1.384 (2) | C25B—C26B | 1.381 (4) |
| C21A—C26A | 1.390 (2) | C25B—H25B | 0.9300 |
| C22A—C23A | 1.400 (3) | C26B—C27B | 1.484 (5) |
| C22A—H22A | 0.9300 | O3X—C20X | 1.202 (12) |
| C23A—C24A | 1.386 (3) | O4X—C27X | 1.190 (8) |
| C23A—H23A | 0.9300 | N2X—C27X | 1.402 (11) |
| C24A—C25A | 1.398 (3) | N2X—C20X | 1.407 (12) |
| C24A—H24A | 0.9300 | C20X—C21X | 1.480 (12) |
| C25A—C26A | 1.382 (2) | C21X—C22X | 1.389 (12) |
| C25A—H25A | 0.9300 | C21X—C26X | 1.395 (12) |
| C26A—C27A | 1.487 (2) | C22X—C23X | 1.410 (13) |
| F1B—C3B | 1.3587 (18) | C22X—H22C | 0.9300 |
| F2B—C16B | 1.357 (2) | C23X—C24X | 1.384 (12) |

| | | | |
|---|---|---|---|
| O1B—C9B | 1.3558 (19) | C23X—H23C | 0.9300 |
| O1B—H1OB | 0.88 (3) | C24X—C25X | 1.400 (9) |
| O2B—C19B | 1.245 (2) | C24X—H24C | 0.9300 |
| N1B—C19B | 1.349 (2) | C25X—C26X | 1.385 (8) |
| N1B—N2B | 1.363 (5) | C25X—H25C | 0.9300 |
| N1B—N2X | 1.432 (11) | C26X—C27X | 1.496 (8) |
| N1B—H1NB | 0.91 (3) | | |

| | | | |
|---|---|---|---|
| C9A—O1A—H1OA | 109 (2) | C2B—C3B—C4B | 123.13 (14) |
| C19A—N1A—N2A | 116.80 (13) | C3B—C4B—C5B | 118.07 (15) |
| C19A—N1A—H1NA | 125.1 (17) | C3B—C4B—H4BA | 121.0 |
| N2A—N1A—H1NA | 118.0 (17) | C5B—C4B—H4BA | 121.0 |
| N1A—N2A—C27A | 122.39 (13) | C4B—C5B—C6B | 120.99 (14) |
| N1A—N2A—C20A | 123.09 (13) | C4B—C5B—H5BA | 119.5 |
| C27A—N2A—C20A | 112.85 (12) | C6B—C5B—H5BA | 119.5 |
| C2A—C1A—C6A | 121.59 (15) | C5B—C6B—C1B | 118.86 (14) |
| C2A—C1A—H1AA | 119.2 | C5B—C6B—C7B | 120.18 (13) |
| C6A—C1A—H1AA | 119.2 | C1B—C6B—C7B | 120.92 (13) |
| C3A—C2A—C1A | 117.94 (15) | C8B—C7B—C12B | 118.82 (14) |
| C3A—C2A—H2AA | 121.0 | C8B—C7B—C6B | 119.80 (13) |
| C1A—C2A—H2AA | 121.0 | C12B—C7B—C6B | 121.34 (13) |
| F1A—C3A—C4A | 118.46 (16) | C7B—C8B—C9B | 120.65 (14) |
| F1A—C3A—C2A | 118.65 (15) | C7B—C8B—H8BA | 119.7 |
| C4A—C3A—C2A | 122.89 (15) | C9B—C8B—H8BA | 119.7 |
| C3A—C4A—C5A | 118.18 (16) | O1B—C9B—C8B | 116.02 (14) |
| C3A—C4A—H4AA | 120.9 | O1B—C9B—C10B | 123.05 (13) |
| C5A—C4A—H4AA | 120.9 | C8B—C9B—C10B | 120.93 (14) |
| C4A—C5A—C6A | 121.40 (15) | C9B—C10B—C11B | 118.48 (13) |
| C4A—C5A—H5AA | 119.3 | C9B—C10B—C19B | 115.99 (13) |
| C6A—C5A—H5AA | 119.3 | C11B—C10B—C19B | 125.53 (13) |
| C1A—C6A—C5A | 117.98 (14) | C12B—C11B—C10B | 118.96 (13) |
| C1A—C6A—C7A | 121.14 (14) | C12B—C11B—C13B | 116.33 (13) |
| C5A—C6A—C7A | 120.89 (14) | C10B—C11B—C13B | 124.69 (13) |
| C8A—C7A—C12A | 117.94 (14) | C11B—C12B—C7B | 122.08 (14) |
| C8A—C7A—C6A | 121.18 (14) | C11B—C12B—H12B | 119.0 |
| C12A—C7A—C6A | 120.83 (13) | C7B—C12B—H12B | 119.0 |
| C7A—C8A—C9A | 121.18 (14) | C18B—C13B—C14B | 118.75 (15) |
| C7A—C8A—H8AA | 119.4 | C18B—C13B—C11B | 119.71 (14) |
| C9A—C8A—H8AA | 119.4 | C14B—C13B—C11B | 121.49 (14) |
| O1A—C9A—C8A | 115.45 (14) | C15B—C14B—C13B | 120.54 (17) |
| O1A—C9A—C10A | 123.68 (14) | C15B—C14B—H14B | 119.7 |
| C8A—C9A—C10A | 120.86 (13) | C13B—C14B—H14B | 119.7 |
| C9A—C10A—C11A | 118.21 (13) | C16B—C15B—C14B | 118.62 (18) |
| C9A—C10A—C19A | 116.23 (13) | C16B—C15B—H15B | 120.7 |
| C11A—C10A—C19A | 125.55 (14) | C14B—C15B—H15B | 120.7 |
| C12A—C11A—C10A | 119.21 (14) | F2B—C16B—C17B | 118.84 (18) |
| C12A—C11A—C13A | 115.87 (13) | F2B—C16B—C15B | 118.30 (18) |
| C10A—C11A—C13A | 124.52 (13) | C17B—C16B—C15B | 122.85 (16) |

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| C11A—C12A—C7A | 122.42 (13) | C16B—C17B—C18B | 117.99 (17) |
| C11A—C12A—H12A | 118.8 | C16B—C17B—H17B | 121.0 |
| C7A—C12A—H12A | 118.8 | C18B—C17B—H17B | 121.0 |
| C14A—C13A—C18A | 118.89 (15) | C17B—C18B—C13B | 121.24 (17) |
| C14A—C13A—C11A | 120.77 (14) | C17B—C18B—H18B | 119.4 |
| C18A—C13A—C11A | 119.99 (14) | C13B—C18B—H18B | 119.4 |
| C13A—C14A—C15A | 120.73 (16) | O2B—C19B—N1B | 119.59 (14) |
| C13A—C14A—H14A | 119.6 | O2B—C19B—C10B | 121.91 (14) |
| C15A—C14A—H14A | 119.6 | N1B—C19B—C10B | 118.46 (14) |
| C16A—C15A—C14A | 118.26 (18) | N1B—N2B—C27B | 124.5 (3) |
| C16A—C15A—H15A | 120.9 | N1B—N2B—C20B | 121.4 (4) |
| C14A—C15A—H15A | 120.9 | C27B—N2B—C20B | 113.4 (4) |
| F2A—C16A—C15A | 118.06 (19) | O3B—C20B—N2B | 127.0 (5) |
| F2A—C16A—C17A | 118.72 (18) | O3B—C20B—C21B | 128.0 (6) |
| C15A—C16A—C17A | 123.20 (16) | N2B—C20B—C21B | 105.0 (4) |
| C16A—C17A—C18A | 118.10 (17) | C22B—C21B—C26B | 119.9 (6) |
| C16A—C17A—H17A | 121.0 | C22B—C21B—C20B | 131.0 (5) |
| C18A—C17A—H17A | 121.0 | C26B—C21B—C20B | 108.5 (4) |
| C17A—C18A—C13A | 120.81 (17) | C21B—C22B—C23B | 118.7 (7) |
| C17A—C18A—H18A | 119.6 | C21B—C22B—H22B | 120.7 |
| C13A—C18A—H18A | 119.6 | C23B—C22B—H22B | 120.7 |
| O2A—C19A—N1A | 119.49 (14) | C24B—C23B—C22B | 121.1 (6) |
| O2A—C19A—C10A | 121.43 (14) | C24B—C23B—H23B | 119.5 |
| N1A—C19A—C10A | 119.00 (13) | C22B—C23B—H23B | 119.5 |
| O3A—C20A—N2A | 124.66 (14) | C23B—C24B—C25B | 121.0 (4) |
| O3A—C20A—C21A | 130.74 (14) | C23B—C24B—H24B | 119.5 |
| N2A—C20A—C21A | 104.60 (13) | C25B—C24B—H24B | 119.5 |
| C22A—C21A—C26A | 121.34 (15) | C26B—C25B—C24B | 117.3 (3) |
| C22A—C21A—C20A | 129.87 (15) | C26B—C25B—H25B | 121.3 |
| C26A—C21A—C20A | 108.77 (13) | C24B—C25B—H25B | 121.3 |
| C21A—C22A—C23A | 117.16 (16) | C25B—C26B—C21B | 121.8 (4) |
| C21A—C22A—H22A | 121.4 | C25B—C26B—C27B | 129.0 (3) |
| C23A—C22A—H22A | 121.4 | C21B—C26B—C27B | 109.2 (3) |
| C24A—C23A—C22A | 121.41 (16) | O4B—C27B—N2B | 125.0 (4) |
| C24A—C23A—H23A | 119.3 | O4B—C27B—C26B | 131.4 (3) |
| C22A—C23A—H23A | 119.3 | N2B—C27B—C26B | 103.6 (3) |
| C23A—C24A—C25A | 121.07 (17) | C27X—N2X—C20X | 113.4 (9) |
| C23A—C24A—H24A | 119.5 | C27X—N2X—N1B | 120.0 (8) |
| C25A—C24A—H24A | 119.5 | C20X—N2X—N1B | 125.5 (9) |
| C26A—C25A—C24A | 117.23 (17) | O3X—C20X—N2X | 119.1 (12) |
| C26A—C25A—H25A | 121.4 | O3X—C20X—C21X | 135.5 (12) |
| C24A—C25A—H25A | 121.4 | N2X—C20X—C21X | 105.2 (9) |
| C25A—C26A—C21A | 121.78 (15) | C22X—C21X—C26X | 122.5 (10) |
| C25A—C26A—C27A | 129.37 (16) | C22X—C21X—C20X | 128.3 (11) |
| C21A—C26A—C27A | 108.85 (14) | C26X—C21X—C20X | 107.4 (9) |
| O4A—C27A—N2A | 125.13 (15) | C21X—C22X—C23X | 115.6 (12) |
| O4A—C27A—C26A | 130.23 (16) | C21X—C22X—H22C | 122.2 |
| N2A—C27A—C26A | 104.65 (13) | C23X—C22X—H22C | 122.2 |

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| C9B—O1B—H1OB | 109 (2) | C24X—C23X—C22X | 121.3 (12) |
| C19B—N1B—N2B | 123.2 (2) | C24X—C23X—H23C | 119.4 |
| C19B—N1B—N2X | 109.5 (3) | C22X—C23X—H23C | 119.4 |
| N2B—N1B—N2X | 13.9 (3) | C23X—C24X—C25X | 122.4 (9) |
| C19B—N1B—H1NB | 122.3 (17) | C23X—C24X—H24C | 118.8 |
| N2B—N1B—H1NB | 114.5 (18) | C25X—C24X—H24C | 118.8 |
| N2X—N1B—H1NB | 128.1 (18) | C26X—C25X—C24X | 116.3 (6) |
| C2B—C1B—C6B | 120.78 (14) | C26X—C25X—H25C | 121.8 |
| C2B—C1B—H1BA | 119.6 | C24X—C25X—H25C | 121.8 |
| C6B—C1B—H1BA | 119.6 | C25X—C26X—C21X | 121.2 (7) |
| C3B—C2B—C1B | 118.16 (14) | C25X—C26X—C27X | 129.2 (6) |
| C3B—C2B—H2BA | 120.9 | C21X—C26X—C27X | 109.4 (7) |
| C1B—C2B—H2BA | 120.9 | O4X—C27X—N2X | 125.7 (7) |
| F1B—C3B—C2B | 118.45 (15) | O4X—C27X—C26X | 130.7 (6) |
| F1B—C3B—C4B | 118.42 (15) | N2X—C27X—C26X | 103.6 (6) |

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| C19A—N1A—N2A—C27A | −76.28 (19) | O1B—C9B—C10B—C11B | −176.72 (15) |
| C19A—N1A—N2A—C20A | 87.92 (18) | C8B—C9B—C10B—C11B | 3.3 (2) |
| C6A—C1A—C2A—C3A | −0.8 (3) | O1B—C9B—C10B—C19B | 3.9 (2) |
| C1A—C2A—C3A—F1A | 179.92 (16) | C8B—C9B—C10B—C19B | −176.07 (15) |
| C1A—C2A—C3A—C4A | −0.1 (3) | C9B—C10B—C11B—C12B | −2.0 (2) |
| F1A—C3A—C4A—C5A | −178.67 (16) | C19B—C10B—C11B—C12B | 177.40 (14) |
| C2A—C3A—C4A—C5A | 1.3 (3) | C9B—C10B—C11B—C13B | 176.17 (15) |
| C3A—C4A—C5A—C6A | −1.7 (3) | C19B—C10B—C11B—C13B | −4.5 (2) |
| C2A—C1A—C6A—C5A | 0.4 (2) | C10B—C11B—C12B—C7B | −0.2 (2) |
| C2A—C1A—C6A—C7A | −179.18 (15) | C13B—C11B—C12B—C7B | −178.43 (15) |
| C4A—C5A—C6A—C1A | 0.9 (2) | C8B—C7B—C12B—C11B | 0.9 (2) |
| C4A—C5A—C6A—C7A | −179.52 (15) | C6B—C7B—C12B—C11B | 178.66 (15) |
| C1A—C6A—C7A—C8A | −162.32 (15) | C12B—C11B—C13B—C18B | −52.7 (2) |
| C5A—C6A—C7A—C8A | 18.1 (2) | C10B—C11B—C13B—C18B | 129.13 (17) |
| C1A—C6A—C7A—C12A | 20.4 (2) | C12B—C11B—C13B—C14B | 124.57 (17) |
| C5A—C6A—C7A—C12A | −159.18 (15) | C10B—C11B—C13B—C14B | −53.6 (2) |
| C12A—C7A—C8A—C9A | 1.3 (2) | C18B—C13B—C14B—C15B | −0.9 (3) |
| C6A—C7A—C8A—C9A | −176.05 (14) | C11B—C13B—C14B—C15B | −178.20 (16) |
| C7A—C8A—C9A—O1A | 176.28 (14) | C13B—C14B—C15B—C16B | 0.3 (3) |
| C7A—C8A—C9A—C10A | −4.6 (2) | C14B—C15B—C16B—F2B | 179.41 (17) |
| O1A—C9A—C10A—C11A | −175.94 (14) | C14B—C15B—C16B—C17B | 0.3 (3) |
| C8A—C9A—C10A—C11A | 5.0 (2) | F2B—C16B—C17B—C18B | −179.42 (16) |
| O1A—C9A—C10A—C19A | 2.9 (2) | C15B—C16B—C17B—C18B | −0.3 (3) |
| C8A—C9A—C10A—C19A | −176.11 (13) | C16B—C17B—C18B—C13B | −0.3 (2) |
| C9A—C10A—C11A—C12A | −2.3 (2) | C14B—C13B—C18B—C17B | 0.9 (2) |
| C19A—C10A—C11A—C12A | 178.97 (14) | C11B—C13B—C18B—C17B | 178.25 (15) |
| C9A—C10A—C11A—C13A | 170.18 (14) | N2B—N1B—C19B—O2B | −4.3 (3) |
| C19A—C10A—C11A—C13A | −8.6 (2) | N2X—N1B—C19B—O2B | −2.1 (5) |
| C10A—C11A—C12A—C7A | −1.0 (2) | N2B—N1B—C19B—C10B | 177.9 (2) |
| C13A—C11A—C12A—C7A | −174.04 (14) | N2X—N1B—C19B—C10B | −179.9 (4) |
| C8A—C7A—C12A—C11A | 1.5 (2) | C9B—C10B—C19B—O2B | −25.2 (2) |
| C6A—C7A—C12A—C11A | 178.84 (14) | C11B—C10B—C19B—O2B | 155.45 (16) |

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| C12A—C11A—C13A—C14A | 128.03 (15) | C9B—C10B—C19B—N1B | 152.55 (15) |
| C10A—C11A—C13A—C14A | −44.6 (2) | C11B—C10B—C19B—N1B | −26.8 (2) |
| C12A—C11A—C13A—C18A | −45.1 (2) | C19B—N1B—N2B—C27B | −91.8 (4) |
| C10A—C11A—C13A—C18A | 142.28 (15) | N2X—N1B—N2B—C27B | −100 (2) |
| C18A—C13A—C14A—C15A | 0.8 (2) | C19B—N1B—N2B—C20B | 77.4 (6) |
| C11A—C13A—C14A—C15A | −172.33 (14) | N2X—N1B—N2B—C20B | 69 (2) |
| C13A—C14A—C15A—C16A | 0.2 (2) | N1B—N2B—C20B—O3B | 3.6 (11) |
| C14A—C15A—C16A—F2A | 177.24 (15) | C27B—N2B—C20B—O3B | 173.9 (7) |
| C14A—C15A—C16A—C17A | −1.1 (3) | N1B—N2B—C20B—C21B | −174.7 (5) |
| F2A—C16A—C17A—C18A | −177.35 (16) | C27B—N2B—C20B—C21B | −4.4 (8) |
| C15A—C16A—C17A—C18A | 1.0 (3) | O3B—C20B—C21B—C22B | 11.1 (18) |
| C16A—C17A—C18A—C13A | 0.1 (3) | N2B—C20B—C21B—C22B | −170.6 (12) |
| C14A—C13A—C18A—C17A | −1.0 (2) | O3B—C20B—C21B—C26B | −178.0 (8) |
| C11A—C13A—C18A—C17A | 172.26 (15) | N2B—C20B—C21B—C26B | 0.2 (8) |
| N2A—N1A—C19A—O2A | −6.3 (2) | C26B—C21B—C22B—C23B | 4.5 (18) |
| N2A—N1A—C19A—C10A | 176.82 (13) | C20B—C21B—C22B—C23B | 174.5 (10) |
| C9A—C10A—C19A—O2A | −32.5 (2) | C21B—C22B—C23B—C24B | −1.0 (18) |
| C11A—C10A—C19A—O2A | 146.25 (16) | C22B—C23B—C24B—C25B | −1.4 (12) |
| C9A—C10A—C19A—N1A | 144.29 (14) | C23B—C24B—C25B—C26B | 0.1 (8) |
| C11A—C10A—C19A—N1A | −36.9 (2) | C24B—C25B—C26B—C21B | 3.5 (8) |
| N1A—N2A—C20A—O3A | 8.2 (2) | C24B—C25B—C26B—C27B | −178.5 (5) |
| C27A—N2A—C20A—O3A | 173.73 (16) | C22B—C21B—C26B—C25B | −5.9 (12) |
| N1A—N2A—C20A—C21A | −171.17 (13) | C20B—C21B—C26B—C25B | −178.0 (6) |
| C27A—N2A—C20A—C21A | −5.62 (17) | C22B—C21B—C26B—C27B | 175.7 (9) |
| O3A—C20A—C21A—C22A | 3.3 (3) | C20B—C21B—C26B—C27B | 3.7 (8) |
| N2A—C20A—C21A—C22A | −177.46 (17) | N1B—N2B—C27B—O4B | −5.8 (7) |
| O3A—C20A—C21A—C26A | −175.39 (18) | C20B—N2B—C27B—O4B | −175.8 (6) |
| N2A—C20A—C21A—C26A | 3.90 (17) | N1B—N2B—C27B—C26B | 176.4 (4) |
| C26A—C21A—C22A—C23A | 0.6 (3) | C20B—N2B—C27B—C26B | 6.4 (6) |
| C20A—C21A—C22A—C23A | −177.93 (17) | C25B—C26B—C27B—O4B | −1.7 (8) |
| C21A—C22A—C23A—C24A | 0.0 (3) | C21B—C26B—C27B—O4B | 176.4 (6) |
| C22A—C23A—C24A—C25A | −0.9 (3) | C25B—C26B—C27B—N2B | 175.8 (5) |
| C23A—C24A—C25A—C26A | 1.1 (3) | C21B—C26B—C27B—N2B | −6.0 (6) |
| C24A—C25A—C26A—C21A | −0.6 (3) | C19B—N1B—N2X—C27X | −90.1 (6) |
| C24A—C25A—C26A—C27A | 178.80 (19) | N2B—N1B—N2X—C27X | 82 (2) |
| C22A—C21A—C26A—C25A | −0.3 (3) | C19B—N1B—N2X—C20X | 102.4 (11) |
| C20A—C21A—C26A—C25A | 178.50 (16) | N2B—N1B—N2X—C20X | −85 (2) |
| C22A—C21A—C26A—C27A | −179.78 (16) | C27X—N2X—C20X—O3X | 179.1 (13) |
| C20A—C21A—C26A—C27A | −0.99 (19) | N1B—N2X—C20X—O3X | −13 (2) |
| N1A—N2A—C27A—O4A | −9.3 (3) | C27X—N2X—C20X—C21X | −5.4 (16) |
| C20A—N2A—C27A—O4A | −174.96 (18) | N1B—N2X—C20X—C21X | 162.9 (10) |
| N1A—N2A—C27A—C26A | 170.70 (14) | O3X—C20X—C21X—C22X | −11 (4) |
| C20A—N2A—C27A—C26A | 5.04 (18) | N2X—C20X—C21X—C22X | 175 (2) |
| C25A—C26A—C27A—O4A | −1.8 (3) | O3X—C20X—C21X—C26X | −176 (2) |
| C21A—C26A—C27A—O4A | 177.7 (2) | N2X—C20X—C21X—C26X | 9.6 (18) |
| C25A—C26A—C27A—N2A | 178.24 (18) | C26X—C21X—C22X—C23X | −9 (3) |
| C21A—C26A—C27A—N2A | −2.32 (19) | C20X—C21X—C22X—C23X | −171.6 (19) |
| C6B—C1B—C2B—C3B | −0.5 (3) | C21X—C22X—C23X—C24X | 3 (3) |

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| C1B—C2B—C3B—F1B | −179.48 (16) | C22X—C23X—C24X—C25X | 3 (2) |
| C1B—C2B—C3B—C4B | 0.9 (3) | C23X—C24X—C25X—C26X | −2.9 (14) |
| F1B—C3B—C4B—C5B | −179.94 (17) | C24X—C25X—C26X—C21X | −2.5 (15) |
| C2B—C3B—C4B—C5B | −0.4 (3) | C24X—C25X—C26X—C27X | −176.2 (8) |
| C3B—C4B—C5B—C6B | −0.7 (3) | C22X—C21X—C26X—C25X | 9 (2) |
| C4B—C5B—C6B—C1B | 1.1 (3) | C20X—C21X—C26X—C25X | 174.8 (11) |
| C4B—C5B—C6B—C7B | 179.01 (17) | C22X—C21X—C26X—C27X | −176.6 (17) |
| C2B—C1B—C6B—C5B | −0.5 (3) | C20X—C21X—C26X—C27X | −10.4 (16) |
| C2B—C1B—C6B—C7B | −178.39 (15) | C20X—N2X—C27X—O4X | 179.8 (11) |
| C5B—C6B—C7B—C8B | −40.4 (2) | N1B—N2X—C27X—O4X | 10.9 (12) |
| C1B—C6B—C7B—C8B | 137.46 (17) | C20X—N2X—C27X—C26X | −0.8 (11) |
| C5B—C6B—C7B—C12B | 141.92 (17) | N1B—N2X—C27X—C26X | −169.7 (5) |
| C1B—C6B—C7B—C12B | −40.2 (2) | C25X—C26X—C27X—O4X | 0.7 (15) |
| C12B—C7B—C8B—C9B | 0.4 (2) | C21X—C26X—C27X—O4X | −173.5 (12) |
| C6B—C7B—C8B—C9B | −177.31 (15) | C25X—C26X—C27X—N2X | −178.7 (8) |
| C7B—C8B—C9B—O1B | 177.45 (16) | C21X—C26X—C27X—N2X | 7.1 (11) |
| C7B—C8B—C9B—C10B | −2.6 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1*A*—H1*NA*···O2*A*$^{i}$ | 0.80 (3) | 2.02 (3) | 2.8000 (19) | 166 (3) |
| O1*B*—H1*OB*···O2*B* | 0.88 (3) | 1.79 (4) | 2.5663 (17) | 145 (4) |
| N1*B*—H1*NB*···O2*B*$^{ii}$ | 0.91 (3) | 2.04 (3) | 2.779 (2) | 138 (2) |
| O1*A*—H1*OA*···O2*A* | 0.82 (3) | 1.94 (3) | 2.6402 (18) | 143 (3) |
| C2*A*—H2*AA*···F2*A*$^{iii}$ | 0.93 | 2.45 | 3.160 (2) | 133 |
| C4*B*—H4*BA*···O3*B*$^{iv}$ | 0.93 | 2.41 | 3.271 (7) | 154 |
| C14*B*—H14*B*···O3*B*$^{v}$ | 0.93 | 2.44 | 3.293 (6) | 152 |
| C25*B*—H25*B*···O1*B*$^{vi}$ | 0.93 | 2.47 | 3.209 (3) | 136 |

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*, *y*+1/2, −*z*+1/2; (iii) *x*, −*y*+1/2, *z*−1/2; (iv) −*x*, −*y*+2, −*z*; (v) −*x*, *y*−1/2, −*z*+1/2; (vi) *x*, −*y*+3/2, *z*+1/2.