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# Ethyl 2-amino-6-(4-bromophenyl)-4-(4-fluorophenyl)cyclohexa-1,3-diene-1-carboxylate

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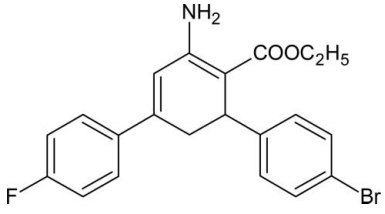
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.051; $wR$ factor = 0.148; data-to-parameter ratio = 15.3.

In the title compound, $C_{21}H_{19}BrFNO_2$, two independent molecules crystallize in the asymmetric unit. The cyclohexa-1,3-diene ring is in a slightly distorted screw-boat conformation. The dihedral angles between the mean planes of the 4-bromophenyl and 4-fluorophenyl rings are 81.0 (3) and 76.4 (2)° in the two independent molecules. In the crystal, N—H···O hydrogen bonds link the molecules into [100] chains.

## Related literature

For cyclohexenones as precursors for functionalized derivatives, see: Samshuddin *et al.* (2013); For 4-bromo-4′-fluorochalcone derivatives, see: Fun *et al.* (2012*a*,*b*,*c*). For related structures, see: Jasinski *et al.* (2012); Kant *et al.* (2012). For puckering parameters, see: Cremer & Pople (1975). For standard bond lengths, see Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{21}H_{19}BrFNO_2$
$M_r$ = 416.28
Monoclinic, $P2_1/n$
$a$ = 9.4599 (2) Å
$b$ = 23.3634 (5) Å
$c$ = 17.2312 (4) Å
$\beta$ = 96.001 (2)°
$V$ = 3787.51 (15) Å$^3$
$Z$ = 8
Cu $K\alpha$ radiation
$\mu$ = 3.16 mm$^{-1}$
$T$ = 173 K
0.32 × 0.28 × 0.22 mm

### Data collection

Agilent Xcalibur (Eos, Gemini) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
$T_{min}$ = 0.587, $T_{max}$ = 1.000
25170 measured reflections
7427 independent reflections
5973 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.148
$S$ = 1.03
7427 reflections
487 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.13 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.53 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1$A$—H1$AA$···O2$A$ | 0.77 (3) | 2.09 (3) | 2.698 (4) | 136 (3) |
| N1$A$—H1$AB$···O2$B^{i}$ | 0.77 (4) | 2.17 (4) | 2.915 (4) | 162 (4) |
| N1$B$—H1$BA$···O2$A^{ii}$ | 0.87 (3) | 2.20 (4) | 3.044 (3) | 163 (3) |
| N1$B$—H1$BB$···O2$B$ | 0.85 (4) | 2.07 (4) | 2.714 (3) | 132 (3) |

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5341).

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# supporting information

*Acta Cryst.* (2013). E**69**, o1473 [doi:10.1107/S1600536813023325]

# Ethyl 2-amino-6-(4-bromophenyl)-4-(4-fluorophenyl)cyclohexa-1,3-diene-1-carboxylate

**B. Narayana, M. Sapnakumari, Jerry P. Jasinski, Peter M. Fraiser and H. S. Yathirajan**

## S1. Comment

Cyclohexenones are well known precursors for various functionalized derivatives such as indazoles, dibenzodiazepines, terphenyls, aminated derivatves etc. (Samshuddin *et al.*, 2013). The title compound, (I), was prepared by the amination of cyclohexenone derivative of 4-bromo-4′-fluorochalcone with ammonium acetate. The crystal structure of a similar aminated product viz., ethyl 2-amino-4,6-bis (4-fluorophenyl)cyclohexa-1,3-diene-1-carboxylate has been reported (Jasinski *et al.*, 2012). Also, the crystal structure of precursor of the title compound (I) viz., ethyl 6-(4-bromophenyl)-4-(4-fluorophenyl)-2-oxocyclohex-3-ene-1-carboxylate has been reported (Kant *et al.*, 2012). In continuation of our work on the synthesis of 4-bromo-4′-fluorochalcone derivatives (Fun *et al.* 2012*a*, 2012*b*, 2012*c*), the title compound (I), $C_{21}H_{19}NO_2FBr$, was prepared and its crystal structure is reported.

In the title compound, $C_{21}H_{19}NO_2FBr$ two independent molecules [A & B]crystallize in the asymmetric unit (Fig. 1). The cyclohexa-1,3-diene ring is in a slightly distorted screw-boat conformation (puckering parameters Q, $\theta$, and $\varphi$ = 0.434 (3)Å, 64.7 (4)°, 271.3 (4)° [A] and 0.355 (3)Å, 63.3 (5)°, 269.7 (6)° [B], respectively; (Cremer & Pople, 1975). Bond lengths are in normal ranges (Allen *et al.*, 1987)). The dihedral angle between the mean planes of the 4-bromophenyl and 4-fluorophenyl rings is 81.0 (3)° [A] and 76.4 (2)° [B]. In the crystal, N—H···O hydrogen bonds form chains along [010] and contribute to packing stability (Fig. 2).

## S2. Experimental

A mixture of ethyl 6-(4-bromophenyl)-4-(4-fluorophenyl)-2-oxocyclohex- 3-ene-1-carboxylate (4.17 g, 0.01 mol) and ammonium acetate (1.54 g, 0.02 mol) in 30 ml glacial acetic acid was refluxed for 6 hours. The reaction mixture was cooled and poured into 50 ml ice-cold water. The precipitate was collected by filtration and purified by recrystallization from ethanol. Single crystals were grown from ethanol by the slow evaporation method. (m.p. 418–420 K).

## S3. Refinement

H1AA, H1AB, H1BA and H1BB were located by a difference map and refined isotropically. All of the remaining H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.95Å (CH) or 0.99° ($CH_2$) or 0.98° ($CH_3$). Isotropic displacement parameters for these atoms were set to 1.2 (CH) or 1.5 (OH) times $U_{eq}$ of the parent atom. Idealised Me refined as rotating group: C1A(H1AC,H1AD,H1AE), C1B(H1BC,H1BD,H1BE).

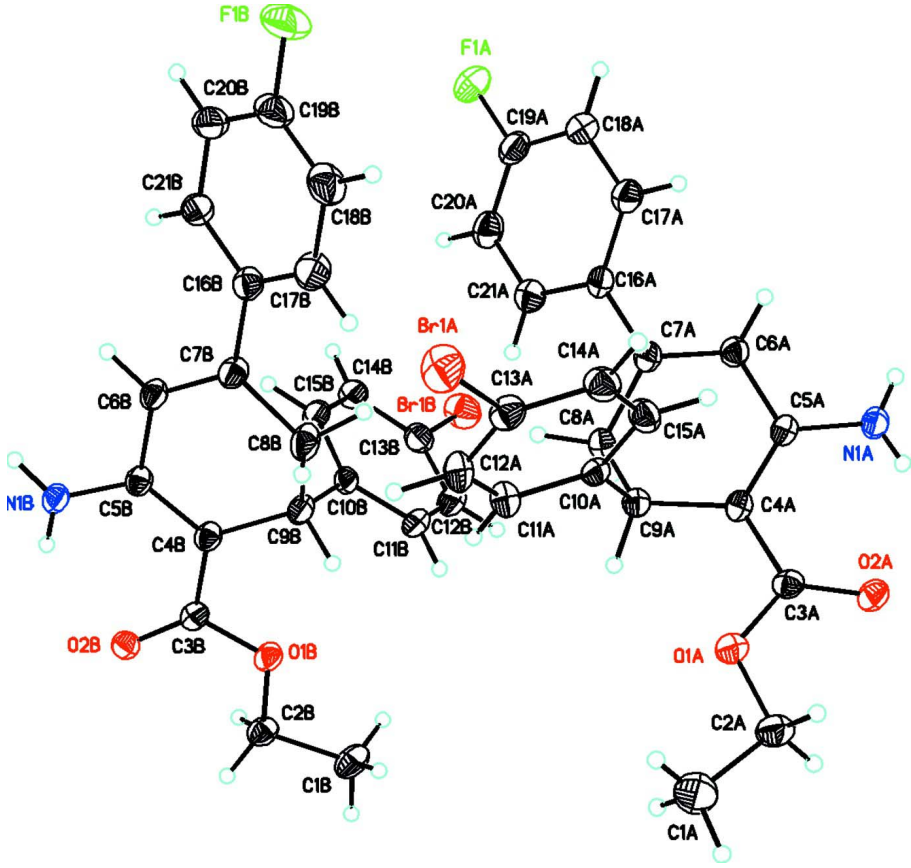


**Figure 1**

Molecular structure of the title compound showing the atom labeling scheme and 30% probability displacement ellipsoids.

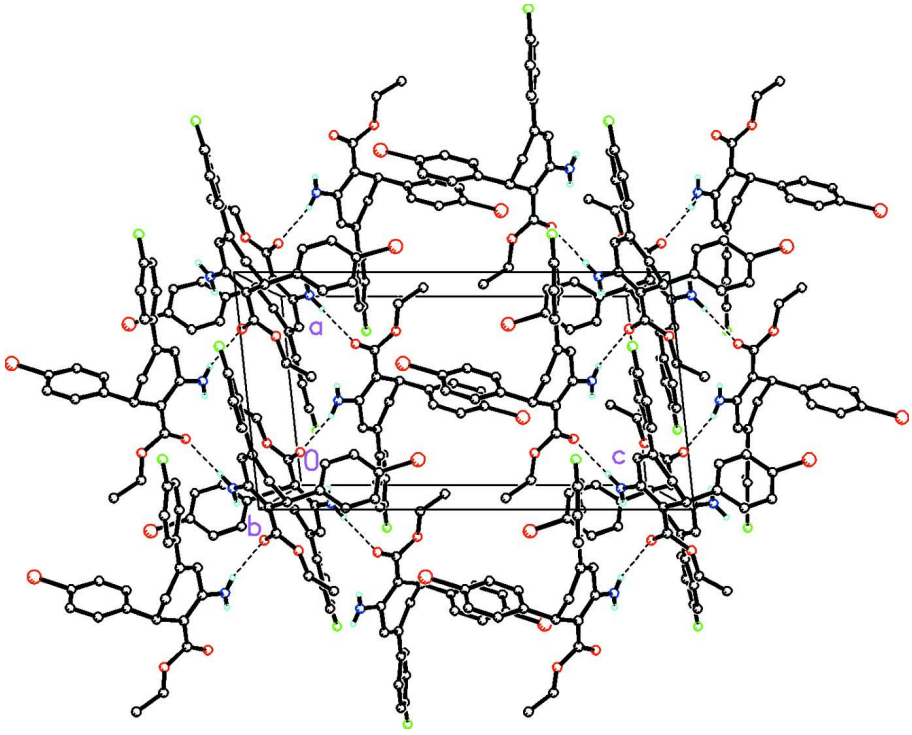


**Figure 2**

Packing diagram of the title compound viewed along the *b* axis. Dashed lines indicate weak N—H···O hydrogen bonds which form chains along [100]. H atoms not involved in these hydrogen bonds have been deleted for clarity.

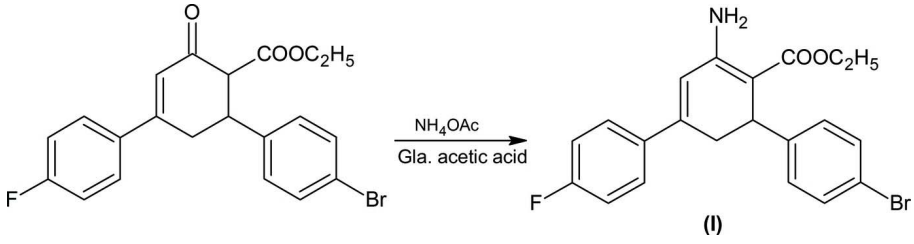


**Figure 3**

Synthesis of (I).

### Ethyl 2-amino-6-(4-bromophenyl)-4-(4-fluorophenyl)cyclohexa-1,3-diene-1-carboxylate

*Crystal data*

$C_{21}H_{19}BrFNO_2$
$M_r = 416.28$
Monoclinic, $P2_1/n$
$a = 9.4599$ (2) Å
$b = 23.3634$ (5) Å
$c = 17.2312$ (4) Å
$\beta = 96.001$ (2)°
$V = 3787.51$ (15) Å$^3$
$Z = 8$

$F(000) = 1696$
$D_x = 1.460$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 7321 reflections
$\theta = 3.2$–72.3°
$\mu = 3.16$ mm$^{-1}$
$T = 173$ K
Irregular, yellow
0.32 × 0.28 × 0.22 mm

*Data collection*

Agilent Xcalibur (Eos, Gemini) diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
$T_{min}$ = 0.587, $T_{max}$ = 1.000
25170 measured reflections
7427 independent reflections
5973 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040
$\theta_{max}$ = 72.5°, $\theta_{min}$ = 3.2°
$h$ = −11→10
$k$ = −28→25
$l$ = −21→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.148
$S$ = 1.03
7427 reflections
487 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0771P)^2 + 2.9658P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.13 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.53 e Å$^{-3}$

*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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1A | 0.37157 (5) | 0.43234 (2) | 0.64815 (2) | 0.05829 (15) |
| F1A | −0.1959 (2) | 0.20568 (10) | 0.24677 (16) | 0.0692 (7) |
| O1A | 0.7906 (2) | 0.41473 (10) | 0.33655 (13) | 0.0414 (5) |
| O2A | 0.7261 (2) | 0.46881 (9) | 0.23026 (12) | 0.0364 (5) |
| N1A | 0.4536 (3) | 0.45651 (12) | 0.16870 (16) | 0.0377 (6) |
| H1AA | 0.523 (4) | 0.4738 (13) | 0.1701 (18) | 0.022 (8)* |
| H1AB | 0.382 (4) | 0.4657 (16) | 0.147 (2) | 0.039 (10)* |
| C1A | 1.0010 (5) | 0.4226 (2) | 0.4216 (3) | 0.0819 (16) |
| H1AC | 1.0218 | 0.3825 | 0.4110 | 0.123* |
| H1AD | 0.9448 | 0.4249 | 0.4662 | 0.123* |
| H1AE | 1.0903 | 0.4436 | 0.4337 | 0.123* |
| C2A | 0.9191 (4) | 0.44839 (17) | 0.3518 (2) | 0.0478 (8) |
| H2AA | 0.8955 | 0.4888 | 0.3620 | 0.057* |
| H2AB | 0.9752 | 0.4471 | 0.3064 | 0.057* |
| C3A | 0.6981 (3) | 0.43038 (12) | 0.27564 (17) | 0.0317 (6) |
| C4A | 0.5687 (3) | 0.39797 (12) | 0.27159 (16) | 0.0315 (6) |
| C5A | 0.4532 (3) | 0.41309 (12) | 0.22021 (16) | 0.0315 (6) |
| C6A | 0.3182 (3) | 0.38225 (13) | 0.22013 (17) | 0.0342 (6) |
| H6A | 0.2340 | 0.3988 | 0.1947 | 0.041* |
| C7A | 0.3106 (3) | 0.33092 (12) | 0.25538 (16) | 0.0325 (6) |

| | | | | |
|---|---|---|---|---|
| C8A | 0.4461 (3) | 0.30516 (12) | 0.29415 (17) | 0.0345 (6) |
| H8AA | 0.4924 | 0.2827 | 0.2552 | 0.041* |
| H8AB | 0.4227 | 0.2786 | 0.3357 | 0.041* |
| C9A | 0.5506 (3) | 0.35068 (12) | 0.32998 (16) | 0.0320 (6) |
| H9A | 0.6451 | 0.3316 | 0.3416 | 0.038* |
| C10A | 0.5058 (3) | 0.37256 (12) | 0.40751 (16) | 0.0303 (6) |
| C11A | 0.5381 (4) | 0.33980 (13) | 0.47408 (18) | 0.0385 (7) |
| H11A | 0.5885 | 0.3049 | 0.4704 | 0.046* |
| C12A | 0.4988 (4) | 0.35662 (14) | 0.54587 (18) | 0.0436 (7) |
| H12A | 0.5218 | 0.3337 | 0.5910 | 0.052* |
| C13A | 0.4255 (3) | 0.40728 (14) | 0.55037 (18) | 0.0388 (7) |
| C14A | 0.3931 (4) | 0.44123 (15) | 0.4856 (2) | 0.0418 (7) |
| H14A | 0.3431 | 0.4762 | 0.4897 | 0.050* |
| C15A | 0.4342 (3) | 0.42383 (14) | 0.41475 (18) | 0.0391 (7) |
| H15A | 0.4130 | 0.4474 | 0.3701 | 0.047* |
| C16A | 0.1765 (3) | 0.29819 (13) | 0.25295 (17) | 0.0348 (6) |
| C17A | 0.0446 (4) | 0.32440 (14) | 0.2399 (2) | 0.0452 (8) |
| H17A | 0.0400 | 0.3646 | 0.2319 | 0.054* |
| C18A | −0.0808 (4) | 0.29345 (16) | 0.2383 (2) | 0.0500 (8) |
| H18A | −0.1703 | 0.3122 | 0.2308 | 0.060* |
| C19A | −0.0729 (4) | 0.23585 (16) | 0.2475 (2) | 0.0472 (8) |
| C20A | 0.0542 (4) | 0.20668 (15) | 0.2570 (2) | 0.0518 (9) |
| H20A | 0.0565 | 0.1661 | 0.2612 | 0.062* |
| C21A | 0.1786 (4) | 0.23819 (14) | 0.2602 (2) | 0.0443 (7) |
| H21A | 0.2674 | 0.2189 | 0.2674 | 0.053* |
| Br1B | 0.32238 (5) | 0.06632 (2) | 0.13555 (2) | 0.06171 (15) |
| F1B | −0.1976 (3) | 0.29436 (12) | 0.58030 (17) | 0.0815 (8) |
| O1B | 0.7450 (2) | 0.08834 (9) | 0.46357 (12) | 0.0365 (5) |
| O2B | 0.7067 (2) | 0.02371 (9) | 0.55597 (12) | 0.0341 (4) |
| N1B | 0.4602 (3) | 0.03596 (11) | 0.62187 (15) | 0.0357 (5) |
| H1BA | 0.394 (4) | 0.0269 (14) | 0.6509 (19) | 0.030 (8)* |
| H1BB | 0.532 (4) | 0.0150 (15) | 0.618 (2) | 0.036 (9)* |
| C1B | 0.9329 (4) | 0.09062 (15) | 0.3842 (2) | 0.0476 (8) |
| H1BC | 0.8671 | 0.0900 | 0.3364 | 0.071* |
| H1BD | 1.0235 | 0.0733 | 0.3740 | 0.071* |
| H1BE | 0.9490 | 0.1303 | 0.4014 | 0.071* |
| C2B | 0.8696 (3) | 0.05690 (13) | 0.4476 (2) | 0.0387 (7) |
| H2BA | 0.8437 | 0.0177 | 0.4292 | 0.046* |
| H2BB | 0.9381 | 0.0542 | 0.4950 | 0.046* |
| C3B | 0.6680 (3) | 0.06649 (12) | 0.51815 (17) | 0.0311 (6) |
| C4B | 0.5413 (3) | 0.09959 (12) | 0.52506 (17) | 0.0322 (6) |
| C5B | 0.4440 (3) | 0.08185 (12) | 0.57450 (17) | 0.0315 (6) |
| C6B | 0.3117 (3) | 0.11419 (12) | 0.57836 (17) | 0.0353 (6) |
| H6B | 0.2381 | 0.0980 | 0.6048 | 0.042* |
| C7B | 0.2919 (3) | 0.16682 (12) | 0.54492 (18) | 0.0367 (6) |
| C8B | 0.4108 (4) | 0.19339 (14) | 0.5065 (2) | 0.0478 (8) |
| H8BA | 0.4680 | 0.2174 | 0.5454 | 0.057* |
| H8BB | 0.3694 | 0.2190 | 0.4643 | 0.057* |

| | | | | |
|---|---|---|---|---|
| C9B | 0.5104 (3) | 0.15061 (12) | 0.47171 (18) | 0.0344 (6) |
| H9B | 0.6029 | 0.1709 | 0.4692 | 0.041* |
| C10B | 0.4599 (3) | 0.13196 (12) | 0.38868 (18) | 0.0338 (6) |
| C11B | 0.5379 (3) | 0.14645 (15) | 0.32743 (19) | 0.0439 (8) |
| H11B | 0.6200 | 0.1698 | 0.3375 | 0.053* |
| C12B | 0.4985 (4) | 0.12771 (17) | 0.2523 (2) | 0.0492 (8) |
| H12B | 0.5529 | 0.1379 | 0.2110 | 0.059* |
| C13B | 0.3789 (4) | 0.09399 (14) | 0.23795 (19) | 0.0425 (7) |
| C14B | 0.2974 (4) | 0.07961 (14) | 0.2971 (2) | 0.0427 (7) |
| H14B | 0.2139 | 0.0571 | 0.2864 | 0.051* |
| C15B | 0.3393 (3) | 0.09842 (13) | 0.3717 (2) | 0.0408 (7) |
| H15B | 0.2843 | 0.0882 | 0.4126 | 0.049* |
| C16B | 0.1623 (3) | 0.20068 (13) | 0.55263 (18) | 0.0383 (7) |
| C17B | 0.1648 (4) | 0.26074 (15) | 0.5510 (2) | 0.0506 (9) |
| H17B | 0.2508 | 0.2799 | 0.5432 | 0.061* |
| C18B | 0.0451 (5) | 0.29259 (17) | 0.5605 (2) | 0.0583 (10) |
| H18B | 0.0479 | 0.3332 | 0.5602 | 0.070* |
| C19B | −0.0789 (4) | 0.26373 (18) | 0.5706 (2) | 0.0545 (9) |
| C20B | −0.0863 (4) | 0.20618 (17) | 0.5734 (2) | 0.0496 (8) |
| H20B | −0.1734 | 0.1877 | 0.5806 | 0.060* |
| C21B | 0.0355 (3) | 0.17440 (14) | 0.56566 (19) | 0.0412 (7) |
| H21B | 0.0319 | 0.1339 | 0.5693 | 0.049* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1A | 0.0728 (3) | 0.0676 (3) | 0.0371 (2) | 0.0088 (2) | 0.01827 (18) | −0.00322 (16) |
| F1A | 0.0491 (12) | 0.0690 (15) | 0.0906 (18) | −0.0199 (11) | 0.0129 (12) | 0.0164 (13) |
| O1A | 0.0323 (11) | 0.0490 (12) | 0.0426 (12) | −0.0040 (9) | 0.0018 (9) | 0.0067 (10) |
| O2A | 0.0354 (11) | 0.0427 (11) | 0.0327 (10) | −0.0033 (9) | 0.0117 (8) | 0.0009 (9) |
| N1A | 0.0364 (15) | 0.0392 (14) | 0.0367 (14) | −0.0076 (13) | −0.0002 (12) | 0.0096 (11) |
| C1A | 0.062 (3) | 0.101 (4) | 0.076 (3) | −0.025 (3) | −0.023 (2) | 0.025 (3) |
| C2A | 0.0348 (17) | 0.057 (2) | 0.050 (2) | −0.0069 (15) | −0.0012 (14) | 0.0017 (16) |
| C3A | 0.0294 (14) | 0.0369 (15) | 0.0303 (14) | 0.0033 (11) | 0.0090 (11) | −0.0031 (11) |
| C4A | 0.0355 (15) | 0.0318 (14) | 0.0280 (13) | −0.0030 (12) | 0.0068 (11) | 0.0012 (11) |
| C5A | 0.0356 (15) | 0.0307 (14) | 0.0290 (14) | −0.0035 (11) | 0.0076 (11) | 0.0007 (11) |
| C6A | 0.0345 (15) | 0.0361 (15) | 0.0316 (14) | −0.0031 (12) | 0.0016 (11) | 0.0028 (11) |
| C7A | 0.0360 (15) | 0.0329 (14) | 0.0287 (14) | −0.0028 (12) | 0.0044 (11) | 0.0001 (11) |
| C8A | 0.0404 (16) | 0.0305 (14) | 0.0320 (14) | −0.0013 (12) | 0.0015 (12) | 0.0031 (11) |
| C9A | 0.0315 (14) | 0.0330 (14) | 0.0313 (14) | −0.0011 (11) | 0.0027 (11) | 0.0031 (11) |
| C10A | 0.0251 (13) | 0.0332 (14) | 0.0325 (14) | −0.0048 (11) | 0.0025 (11) | 0.0024 (11) |
| C11A | 0.0459 (17) | 0.0357 (15) | 0.0339 (15) | 0.0017 (13) | 0.0038 (13) | 0.0040 (12) |
| C12A | 0.056 (2) | 0.0441 (17) | 0.0304 (15) | 0.0007 (15) | 0.0056 (14) | 0.0080 (13) |
| C13A | 0.0393 (16) | 0.0478 (17) | 0.0303 (15) | −0.0025 (14) | 0.0080 (12) | −0.0032 (13) |
| C14A | 0.0397 (17) | 0.0468 (18) | 0.0393 (17) | 0.0067 (14) | 0.0061 (13) | −0.0005 (13) |
| C15A | 0.0404 (17) | 0.0451 (17) | 0.0315 (15) | 0.0060 (13) | 0.0018 (12) | 0.0059 (12) |
| C16A | 0.0393 (16) | 0.0341 (15) | 0.0314 (14) | −0.0049 (12) | 0.0050 (12) | 0.0039 (11) |
| C17A | 0.0445 (18) | 0.0381 (16) | 0.054 (2) | −0.0030 (14) | 0.0088 (15) | 0.0052 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C18A | 0.0397 (18) | 0.056 (2) | 0.056 (2) | 0.0000 (15) | 0.0092 (15) | 0.0112 (17) |
| C19A | 0.0426 (18) | 0.053 (2) | 0.0471 (19) | −0.0129 (15) | 0.0082 (15) | 0.0070 (15) |
| C20A | 0.058 (2) | 0.0392 (18) | 0.059 (2) | −0.0102 (16) | 0.0086 (17) | 0.0055 (15) |
| C21A | 0.0453 (18) | 0.0407 (17) | 0.0469 (18) | −0.0027 (14) | 0.0053 (14) | 0.0029 (14) |
| Br1B | 0.0622 (3) | 0.0741 (3) | 0.0478 (2) | 0.0055 (2) | 0.00066 (19) | −0.00554 (18) |
| F1B | 0.0622 (15) | 0.0926 (19) | 0.0917 (19) | 0.0427 (14) | 0.0173 (14) | 0.0110 (15) |
| O1B | 0.0350 (11) | 0.0394 (11) | 0.0377 (11) | 0.0048 (9) | 0.0154 (9) | 0.0039 (9) |
| O2B | 0.0336 (10) | 0.0355 (10) | 0.0332 (10) | 0.0024 (8) | 0.0039 (8) | 0.0014 (8) |
| N1B | 0.0362 (13) | 0.0371 (13) | 0.0358 (13) | 0.0046 (11) | 0.0140 (11) | 0.0068 (10) |
| C1B | 0.0456 (18) | 0.0488 (19) | 0.052 (2) | −0.0019 (15) | 0.0248 (16) | −0.0068 (16) |
| C2B | 0.0348 (15) | 0.0390 (16) | 0.0440 (17) | 0.0022 (13) | 0.0127 (13) | −0.0027 (13) |
| C3B | 0.0321 (14) | 0.0334 (14) | 0.0283 (14) | −0.0037 (11) | 0.0057 (11) | −0.0051 (11) |
| C4B | 0.0351 (15) | 0.0297 (14) | 0.0332 (14) | 0.0009 (12) | 0.0106 (11) | −0.0002 (11) |
| C5B | 0.0356 (15) | 0.0300 (13) | 0.0299 (14) | −0.0001 (11) | 0.0081 (11) | −0.0007 (11) |
| C6B | 0.0390 (16) | 0.0334 (14) | 0.0359 (15) | 0.0025 (12) | 0.0150 (12) | 0.0038 (12) |
| C7B | 0.0390 (16) | 0.0303 (14) | 0.0430 (16) | 0.0029 (12) | 0.0144 (13) | 0.0004 (12) |
| C8B | 0.058 (2) | 0.0322 (16) | 0.058 (2) | 0.0094 (15) | 0.0280 (17) | 0.0110 (14) |
| C9B | 0.0356 (15) | 0.0287 (14) | 0.0415 (16) | 0.0016 (12) | 0.0160 (12) | 0.0051 (12) |
| C10B | 0.0326 (14) | 0.0303 (14) | 0.0403 (16) | 0.0085 (11) | 0.0120 (12) | 0.0120 (12) |
| C11B | 0.0329 (15) | 0.057 (2) | 0.0435 (18) | −0.0055 (14) | 0.0102 (13) | 0.0132 (15) |
| C12B | 0.0404 (18) | 0.068 (2) | 0.0408 (18) | −0.0018 (16) | 0.0120 (14) | 0.0133 (16) |
| C13B | 0.0422 (17) | 0.0464 (17) | 0.0391 (17) | 0.0081 (14) | 0.0045 (13) | 0.0049 (14) |
| C14B | 0.0372 (16) | 0.0399 (16) | 0.0515 (19) | −0.0001 (13) | 0.0075 (14) | 0.0062 (14) |
| C15B | 0.0378 (16) | 0.0385 (16) | 0.0482 (18) | 0.0005 (13) | 0.0148 (14) | 0.0095 (13) |
| C16B | 0.0437 (17) | 0.0360 (15) | 0.0367 (16) | 0.0048 (13) | 0.0112 (13) | 0.0015 (12) |
| C17B | 0.055 (2) | 0.0398 (17) | 0.059 (2) | 0.0078 (16) | 0.0197 (17) | 0.0024 (15) |
| C18B | 0.071 (3) | 0.046 (2) | 0.060 (2) | 0.0206 (19) | 0.015 (2) | 0.0042 (17) |
| C19B | 0.051 (2) | 0.067 (2) | 0.047 (2) | 0.0254 (19) | 0.0099 (16) | 0.0043 (17) |
| C20B | 0.0385 (17) | 0.070 (2) | 0.0410 (18) | 0.0084 (16) | 0.0059 (14) | 0.0041 (16) |
| C21B | 0.0407 (17) | 0.0443 (17) | 0.0391 (16) | 0.0046 (14) | 0.0073 (13) | 0.0021 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1A—C13A | 1.903 (3) | Br1B—C13B | 1.903 (3) |
| F1A—C19A | 1.359 (4) | F1B—C19B | 1.357 (4) |
| O1A—C2A | 1.449 (4) | O1B—C2B | 1.439 (4) |
| O1A—C3A | 1.345 (4) | O1B—C3B | 1.348 (3) |
| O2A—C3A | 1.237 (4) | O2B—C3B | 1.228 (4) |
| N1A—H1AA | 0.77 (3) | N1B—H1BA | 0.87 (3) |
| N1A—H1AB | 0.77 (4) | N1B—H1BB | 0.85 (4) |
| N1A—C5A | 1.348 (4) | N1B—C5B | 1.346 (4) |
| C1A—H1AC | 0.9800 | C1B—H1BC | 0.9800 |
| C1A—H1AD | 0.9800 | C1B—H1BD | 0.9800 |
| C1A—H1AE | 0.9800 | C1B—H1BE | 0.9800 |
| C1A—C2A | 1.489 (6) | C1B—C2B | 1.519 (4) |
| C2A—H2AA | 0.9900 | C2B—H2BA | 0.9900 |
| C2A—H2AB | 0.9900 | C2B—H2BB | 0.9900 |
| C3A—C4A | 1.434 (4) | C3B—C4B | 1.442 (4) |

| | | | |
|---|---|---|---|
| C4A—C5A | 1.379 (4) | C4B—C5B | 1.382 (4) |
| C4A—C9A | 1.516 (4) | C4B—C9B | 1.515 (4) |
| C5A—C6A | 1.466 (4) | C5B—C6B | 1.469 (4) |
| C6A—H6A | 0.9500 | C6B—H6B | 0.9500 |
| C6A—C7A | 1.350 (4) | C6B—C7B | 1.363 (4) |
| C7A—C8A | 1.507 (4) | C7B—C8B | 1.498 (4) |
| C7A—C16A | 1.478 (4) | C7B—C16B | 1.477 (4) |
| C8A—H8AA | 0.9900 | C8B—H8BA | 0.9900 |
| C8A—H8AB | 0.9900 | C8B—H8BB | 0.9900 |
| C8A—C9A | 1.537 (4) | C8B—C9B | 1.537 (4) |
| C9A—H9A | 1.0000 | C9B—H9B | 1.0000 |
| C9A—C10A | 1.531 (4) | C9B—C10B | 1.524 (4) |
| C10A—C11A | 1.386 (4) | C10B—C11B | 1.391 (4) |
| C10A—C15A | 1.388 (4) | C10B—C15B | 1.389 (4) |
| C11A—H11A | 0.9500 | C11B—H11B | 0.9500 |
| C11A—C12A | 1.385 (4) | C11B—C12B | 1.381 (5) |
| C12A—H12A | 0.9500 | C12B—H12B | 0.9500 |
| C12A—C13A | 1.378 (5) | C12B—C13B | 1.379 (5) |
| C13A—C14A | 1.377 (5) | C13B—C14B | 1.382 (5) |
| C14A—H14A | 0.9500 | C14B—H14B | 0.9500 |
| C14A—C15A | 1.381 (5) | C14B—C15B | 1.377 (5) |
| C15A—H15A | 0.9500 | C15B—H15B | 0.9500 |
| C16A—C17A | 1.388 (5) | C16B—C17B | 1.404 (5) |
| C16A—C21A | 1.407 (4) | C16B—C21B | 1.387 (5) |
| C17A—H17A | 0.9500 | C17B—H17B | 0.9500 |
| C17A—C18A | 1.387 (5) | C17B—C18B | 1.379 (5) |
| C18A—H18A | 0.9500 | C18B—H18B | 0.9500 |
| C18A—C19A | 1.356 (5) | C18B—C19B | 1.379 (6) |
| C19A—C20A | 1.378 (5) | C19B—C20B | 1.348 (6) |
| C20A—H20A | 0.9500 | C20B—H20B | 0.9500 |
| C20A—C21A | 1.384 (5) | C20B—C21B | 1.389 (5) |
| C21A—H21A | 0.9500 | C21B—H21B | 0.9500 |

| | | | |
|---|---|---|---|
| C3A—O1A—C2A | 117.3 (2) | C3B—O1B—C2B | 116.9 (2) |
| H1AA—N1A—H1AB | 125 (4) | H1BA—N1B—H1BB | 122 (3) |
| C5A—N1A—H1AA | 116 (2) | C5B—N1B—H1BA | 120 (2) |
| C5A—N1A—H1AB | 118 (3) | C5B—N1B—H1BB | 117 (2) |
| H1AC—C1A—H1AD | 109.5 | H1BC—C1B—H1BD | 109.5 |
| H1AC—C1A—H1AE | 109.5 | H1BC—C1B—H1BE | 109.5 |
| H1AD—C1A—H1AE | 109.5 | H1BD—C1B—H1BE | 109.5 |
| C2A—C1A—H1AC | 109.5 | C2B—C1B—H1BC | 109.5 |
| C2A—C1A—H1AD | 109.5 | C2B—C1B—H1BD | 109.5 |
| C2A—C1A—H1AE | 109.5 | C2B—C1B—H1BE | 109.5 |
| O1A—C2A—C1A | 106.4 (3) | O1B—C2B—C1B | 105.4 (3) |
| O1A—C2A—H2AA | 110.4 | O1B—C2B—H2BA | 110.7 |
| O1A—C2A—H2AB | 110.4 | O1B—C2B—H2BB | 110.7 |
| C1A—C2A—H2AA | 110.4 | C1B—C2B—H2BA | 110.7 |
| C1A—C2A—H2AB | 110.4 | C1B—C2B—H2BB | 110.7 |

| | | | |
|---|---|---|---|
| H2AA—C2A—H2AB | 108.6 | H2BA—C2B—H2BB | 108.8 |
| O1A—C3A—C4A | 112.1 (2) | O1B—C3B—C4B | 111.6 (2) |
| O2A—C3A—O1A | 121.7 (3) | O2B—C3B—O1B | 121.7 (3) |
| O2A—C3A—C4A | 126.2 (3) | O2B—C3B—C4B | 126.7 (3) |
| C3A—C4A—C9A | 120.5 (3) | C3B—C4B—C9B | 118.8 (2) |
| C5A—C4A—C3A | 120.7 (3) | C5B—C4B—C3B | 120.2 (3) |
| C5A—C4A—C9A | 118.4 (3) | C5B—C4B—C9B | 120.7 (3) |
| N1A—C5A—C4A | 124.0 (3) | N1B—C5B—C4B | 124.9 (3) |
| N1A—C5A—C6A | 115.6 (3) | N1B—C5B—C6B | 115.2 (3) |
| C4A—C5A—C6A | 120.4 (3) | C4B—C5B—C6B | 119.9 (3) |
| C5A—C6A—H6A | 119.2 | C5B—C6B—H6B | 119.2 |
| C7A—C6A—C5A | 121.5 (3) | C7B—C6B—C5B | 121.7 (3) |
| C7A—C6A—H6A | 119.2 | C7B—C6B—H6B | 119.2 |
| C6A—C7A—C8A | 118.2 (3) | C6B—C7B—C8B | 119.0 (3) |
| C6A—C7A—C16A | 122.2 (3) | C6B—C7B—C16B | 121.6 (3) |
| C16A—C7A—C8A | 119.6 (3) | C16B—C7B—C8B | 119.1 (3) |
| C7A—C8A—H8AA | 109.1 | C7B—C8B—H8BA | 108.5 |
| C7A—C8A—H8AB | 109.1 | C7B—C8B—H8BB | 108.5 |
| C7A—C8A—C9A | 112.5 (2) | C7B—C8B—C9B | 115.0 (3) |
| H8AA—C8A—H8AB | 107.8 | H8BA—C8B—H8BB | 107.5 |
| C9A—C8A—H8AA | 109.1 | C9B—C8B—H8BA | 108.5 |
| C9A—C8A—H8AB | 109.1 | C9B—C8B—H8BB | 108.5 |
| C4A—C9A—C8A | 110.5 (2) | C4B—C9B—C8B | 111.3 (2) |
| C4A—C9A—H9A | 107.3 | C4B—C9B—H9B | 106.5 |
| C4A—C9A—C10A | 113.4 (2) | C4B—C9B—C10B | 111.5 (2) |
| C8A—C9A—H9A | 107.3 | C8B—C9B—H9B | 106.5 |
| C10A—C9A—C8A | 110.9 (2) | C10B—C9B—C8B | 114.0 (3) |
| C10A—C9A—H9A | 107.3 | C10B—C9B—H9B | 106.5 |
| C11A—C10A—C9A | 118.7 (3) | C11B—C10B—C9B | 120.2 (3) |
| C11A—C10A—C15A | 118.0 (3) | C15B—C10B—C9B | 121.9 (3) |
| C15A—C10A—C9A | 123.3 (3) | C15B—C10B—C11B | 117.8 (3) |
| C10A—C11A—H11A | 119.1 | C10B—C11B—H11B | 119.3 |
| C12A—C11A—C10A | 121.7 (3) | C12B—C11B—C10B | 121.5 (3) |
| C12A—C11A—H11A | 119.1 | C12B—C11B—H11B | 119.3 |
| C11A—C12A—H12A | 120.7 | C11B—C12B—H12B | 120.5 |
| C13A—C12A—C11A | 118.5 (3) | C13B—C12B—C11B | 119.0 (3) |
| C13A—C12A—H12A | 120.7 | C13B—C12B—H12B | 120.5 |
| C12A—C13A—Br1A | 119.8 (2) | C12B—C13B—Br1B | 120.4 (3) |
| C14A—C13A—Br1A | 118.8 (2) | C12B—C13B—C14B | 121.2 (3) |
| C14A—C13A—C12A | 121.3 (3) | C14B—C13B—Br1B | 118.5 (3) |
| C13A—C14A—H14A | 120.4 | C13B—C14B—H14B | 120.6 |
| C13A—C14A—C15A | 119.2 (3) | C15B—C14B—C13B | 118.8 (3) |
| C15A—C14A—H14A | 120.4 | C15B—C14B—H14B | 120.6 |
| C10A—C15A—H15A | 119.4 | C10B—C15B—H15B | 119.1 |
| C14A—C15A—C10A | 121.2 (3) | C14B—C15B—C10B | 121.8 (3) |
| C14A—C15A—H15A | 119.4 | C14B—C15B—H15B | 119.1 |
| C17A—C16A—C7A | 122.1 (3) | C17B—C16B—C7B | 121.2 (3) |
| C17A—C16A—C21A | 117.3 (3) | C21B—C16B—C7B | 121.2 (3) |

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|---|---|---|---|
| C21A—C16A—C7A | 120.6 (3) | C21B—C16B—C17B | 117.5 (3) |
| C16A—C17A—H17A | 119.1 | C16B—C17B—H17B | 119.3 |
| C18A—C17A—C16A | 121.8 (3) | C18B—C17B—C16B | 121.4 (4) |
| C18A—C17A—H17A | 119.1 | C18B—C17B—H17B | 119.3 |
| C17A—C18A—H18A | 120.7 | C17B—C18B—H18B | 121.0 |
| C19A—C18A—C17A | 118.6 (3) | C17B—C18B—C19B | 118.1 (4) |
| C19A—C18A—H18A | 120.7 | C19B—C18B—H18B | 121.0 |
| F1A—C19A—C20A | 118.7 (3) | F1B—C19B—C18B | 118.9 (4) |
| C18A—C19A—F1A | 118.5 (3) | C20B—C19B—F1B | 118.3 (4) |
| C18A—C19A—C20A | 122.8 (3) | C20B—C19B—C18B | 122.7 (3) |
| C19A—C20A—H20A | 121.0 | C19B—C20B—H20B | 120.6 |
| C19A—C20A—C21A | 118.0 (3) | C19B—C20B—C21B | 118.9 (3) |
| C21A—C20A—H20A | 121.0 | C21B—C20B—H20B | 120.6 |
| C16A—C21A—H21A | 119.3 | C16B—C21B—C20B | 121.3 (3) |
| C20A—C21A—C16A | 121.5 (3) | C16B—C21B—H21B | 119.3 |
| C20A—C21A—H21A | 119.3 | C20B—C21B—H21B | 119.3 |
| | | | |
| Br1A—C13A—C14A—C15A | 178.8 (3) | Br1B—C13B—C14B—C15B | 178.6 (2) |
| F1A—C19A—C20A—C21A | −177.9 (3) | F1B—C19B—C20B—C21B | −178.3 (3) |
| O1A—C3A—C4A—C5A | 170.7 (3) | O1B—C3B—C4B—C5B | 175.9 (3) |
| O1A—C3A—C4A—C9A | −2.3 (4) | O1B—C3B—C4B—C9B | 1.7 (4) |
| O2A—C3A—C4A—C5A | −8.9 (5) | O2B—C3B—C4B—C5B | −4.6 (5) |
| O2A—C3A—C4A—C9A | 178.1 (3) | O2B—C3B—C4B—C9B | −178.8 (3) |
| N1A—C5A—C6A—C7A | 165.1 (3) | N1B—C5B—C6B—C7B | 168.0 (3) |
| C2A—O1A—C3A—O2A | 6.0 (4) | C2B—O1B—C3B—O2B | 4.4 (4) |
| C2A—O1A—C3A—C4A | −173.7 (3) | C2B—O1B—C3B—C4B | −176.1 (2) |
| C3A—O1A—C2A—C1A | 179.5 (3) | C3B—O1B—C2B—C1B | 179.4 (3) |
| C3A—C4A—C5A—N1A | 3.0 (5) | C3B—C4B—C5B—N1B | 3.5 (5) |
| C3A—C4A—C5A—C6A | −175.7 (3) | C3B—C4B—C5B—C6B | −176.9 (3) |
| C3A—C4A—C9A—C8A | −152.6 (3) | C3B—C4B—C9B—C8B | −157.6 (3) |
| C3A—C4A—C9A—C10A | 82.2 (3) | C3B—C4B—C9B—C10B | 73.9 (3) |
| C4A—C5A—C6A—C7A | −16.0 (4) | C4B—C5B—C6B—C7B | −11.6 (5) |
| C4A—C9A—C10A—C11A | −155.2 (3) | C4B—C9B—C10B—C11B | −118.5 (3) |
| C4A—C9A—C10A—C15A | 24.8 (4) | C4B—C9B—C10B—C15B | 58.9 (4) |
| C5A—C4A—C9A—C8A | 34.3 (4) | C5B—C4B—C9B—C8B | 28.3 (4) |
| C5A—C4A—C9A—C10A | −90.9 (3) | C5B—C4B—C9B—C10B | −100.2 (3) |
| C5A—C6A—C7A—C8A | −1.0 (4) | C5B—C6B—C7B—C8B | −2.8 (5) |
| C5A—C6A—C7A—C16A | −177.4 (3) | C5B—C6B—C7B—C16B | −176.5 (3) |
| C6A—C7A—C8A—C9A | 33.8 (4) | C6B—C7B—C8B—C9B | 29.7 (5) |
| C6A—C7A—C16A—C17A | −23.2 (5) | C6B—C7B—C16B—C17B | 151.0 (3) |
| C6A—C7A—C16A—C21A | 153.7 (3) | C6B—C7B—C16B—C21B | −25.7 (5) |
| C7A—C8A—C9A—C4A | −48.8 (3) | C7B—C8B—C9B—C4B | −40.7 (4) |
| C7A—C8A—C9A—C10A | 77.8 (3) | C7B—C8B—C9B—C10B | 86.4 (4) |
| C7A—C16A—C17A—C18A | −179.5 (3) | C7B—C16B—C17B—C18B | −178.0 (3) |
| C7A—C16A—C21A—C20A | −179.1 (3) | C7B—C16B—C21B—C20B | 179.6 (3) |
| C8A—C7A—C16A—C17A | 160.5 (3) | C8B—C7B—C16B—C17B | −22.7 (5) |
| C8A—C7A—C16A—C21A | −22.6 (4) | C8B—C7B—C16B—C21B | 160.6 (3) |
| C8A—C9A—C10A—C11A | 79.9 (3) | C8B—C9B—C10B—C11B | 114.5 (3) |

| | | | |
|---|---|---|---|
| C8A—C9A—C10A—C15A | −100.2 (3) | C8B—C9B—C10B—C15B | −68.1 (4) |
| C9A—C4A—C5A—N1A | 176.1 (3) | C9B—C4B—C5B—N1B | 177.6 (3) |
| C9A—C4A—C5A—C6A | −2.7 (4) | C9B—C4B—C5B—C6B | −2.9 (4) |
| C9A—C10A—C11A—C12A | −179.0 (3) | C9B—C10B—C11B—C12B | 176.7 (3) |
| C9A—C10A—C15A—C14A | 178.5 (3) | C9B—C10B—C15B—C14B | −177.2 (3) |
| C10A—C11A—C12A—C13A | 0.1 (5) | C10B—C11B—C12B—C13B | 0.1 (5) |
| C11A—C10A—C15A—C14A | −1.5 (5) | C11B—C10B—C15B—C14B | 0.3 (5) |
| C11A—C12A—C13A—Br1A | −179.3 (3) | C11B—C12B—C13B—Br1B | −179.1 (3) |
| C11A—C12A—C13A—C14A | −0.9 (5) | C11B—C12B—C13B—C14B | 1.0 (5) |
| C12A—C13A—C14A—C15A | 0.5 (5) | C12B—C13B—C14B—C15B | −1.5 (5) |
| C13A—C14A—C15A—C10A | 0.8 (5) | C13B—C14B—C15B—C10B | 0.8 (5) |
| C15A—C10A—C11A—C12A | 1.0 (5) | C15B—C10B—C11B—C12B | −0.8 (5) |
| C16A—C7A—C8A—C9A | −149.8 (3) | C16B—C7B—C8B—C9B | −156.5 (3) |
| C16A—C17A—C18A—C19A | −1.9 (6) | C16B—C17B—C18B—C19B | −0.9 (6) |
| C17A—C16A—C21A—C20A | −2.0 (5) | C17B—C16B—C21B—C20B | 2.8 (5) |
| C17A—C18A—C19A—F1A | 179.2 (3) | C17B—C18B—C19B—F1B | 179.8 (4) |
| C17A—C18A—C19A—C20A | −1.2 (6) | C17B—C18B—C19B—C20B | 1.7 (6) |
| C18A—C19A—C20A—C21A | 2.6 (6) | C18B—C19B—C20B—C21B | −0.2 (6) |
| C19A—C20A—C21A—C16A | −0.9 (5) | C19B—C20B—C21B—C16B | −2.1 (5) |
| C21A—C16A—C17A—C18A | 3.5 (5) | C21B—C16B—C17B—C18B | −1.2 (6) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1*A*—H1*AA*···O2*A* | 0.77 (3) | 2.09 (3) | 2.698 (4) | 136 (3) |
| N1*A*—H1*AB*···O2*B*$^{i}$ | 0.77 (4) | 2.17 (4) | 2.915 (4) | 162 (4) |
| N1*B*—H1*BA*···O2*A*$^{ii}$ | 0.87 (3) | 2.20 (4) | 3.044 (3) | 163 (3) |
| N1*B*—H1*BB*···O2*B* | 0.85 (4) | 2.07 (4) | 2.714 (3) | 132 (3) |

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