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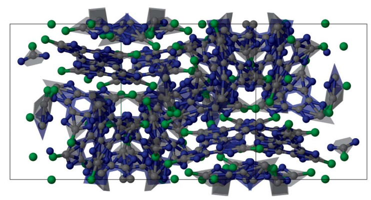
2,6,10-Trichlorotris[1,2,4]triazolo[1,5-*a*:1′,5′-*c*:1″,5″-e][1,3,5]triazine

Daniel Limbach, Heiner Detert* and Dieter Schollmeyer

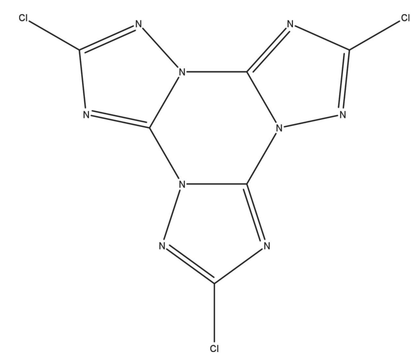
University of Mainz, Institut of Organic Chemistry, Duesbergweg 10-14, 55099 Mainz, Germany. *Correspondence e-mail: detert@uni-mainz.de

Three very similar and nearly planar molecules are present in the asymmetric unit of the title compound, $C_6Cl_3N_9$. Whereas the threefold 1,5-annulation of the chlorotriazole moieties is obvious, all of the C and N atoms in the central triazine ring are equally disordered on the same site, approaching D_{3h} symmetry for each of the molecules.

3D view



Chemical scheme



Structure description

Tristriazolotriazine (TTT) prepared according to the Huisgen route (Huisgen *et al.*, 1960) is a new core for discotic liquid crystals (Cristiano *et al.*, 2008; Glang *et al.*, 2014; Rieth *et al.*, 2014, 2015). These compounds suffer a thermal isomerization (Rieth *et al.*, 2018) of all annulated triazole moieties from the original 4,3-annulation to the 1,5-annulation, like in the title compound. The title compound, $C_6N_9Cl_3$, was prepared for the first time by Tartakovsky *et al.* (2005). The current study reports the first crystal structure determination of a TTT without carbon substituents.

The monoclinic unit cell comprises of three independent but very similar molecules (*A*–*C*). All of them are nearly planar, the maximum deviation from the least-squares plane being 0.1029 (14) Å at N2*A* for molecule *A*. As a result of the disorder of all carbon and nitrogen atoms in the central triazine ring, the expected C_{3v} point group symmetry with alternating C, N atoms is not observed. Instead, the disorder of the triazine ring leads to an apparently higher symmetry approaching point group D_{3h}. Atoms *X* in Fig. 1 represent carbon and nitrogen sites with a statistical occupation. Nevertheless, the bond lengths in the triazine ring are alternating. Representative for all molecules corresponding bond lengths in molecule *A* are: $X8—X9$ = 1.370 (2) Å, $X13—X14$ = 1.373 (2) Å, and $X3—X4$ = 1.370 (2) Å, whereas the 1,5-bonds are shorter with $X9—X13$ = 1.355 (2) Å, $X14—X3$ = 1.359 (2) Å and $X4—X8$ = 1.359 (2) Å. With values between 1.692 (2) and 1.698 (2) Å, the C—Cl bonds are comparatively short. As a result of missing

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_6Cl_3N_9$
M_r	304.50
Crystal system, space group	Monoclinic, *I*2/*a*
Temperature (K)	193
a, *b*, *c* (Å)	22.2914 (8), 14.1339 (3), 23.1869 (8)
β (°)	115.732 (2)
V (Å^3)	6580.9 (4)
Z	24
Radiation type	Mo *K*α
μ (mm^{-1})	0.83
Crystal size (mm)	0.30 × 0.28 × 0.18
Data collection	
Diffractometer	Stoe IPDS 2T
Absorption correction	Integration (*X-RED* and *X-SHAPE*; Stoe, 2006)
T_{min}, T_{max}	0.769, 0.877
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18928, 8167, 6939
R_{int}	0.020
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.086, 1.06
No. of reflections	8167
No. of parameters	496
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.46

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2006), *SIR2004* (Altomare *et al.*, 1999), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2015) and *publCIF* (Westrip, 2010).

hydrogen atoms and the twisted orientation of the molecules to each other, hydrogen-bonding interactions and π–π stacking are impossible. Therefore the cohesion of the crystal appears to be caused by van der Waals forces alone.

Synthesis and crystallization

A reaction tube was filled with 1.5 g (7.2 mmol) 3,5-dichloro-(1,2,4)-triazole and heated for 10 min to 483 K, 15 min to 513 K and finally 25 min to 553 K. The reaction was controlled *via* evolution of hydrogen chloride. The crude product was dissolved in chloroform, mixed with silica gel (7 g) and purified by chromatography on silica using toluene/petroleum ether (6/1 *v*/*v*) as an eluent. 170 mg (23%) of a colourless product with ^{13}C: 144.49, 155.63 (DMSO-d_6), IR: 706, 1226, 1270, 1627 cm^{-1}, and m/z = 302 were obtained. Recrystallization from chloroform yielded colourless crystals with m.p. 587 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The sequence of the C and N atoms in the central triazine ring of each molecule (*A*–*C*) could not be determined. Hence all sites were refined with half

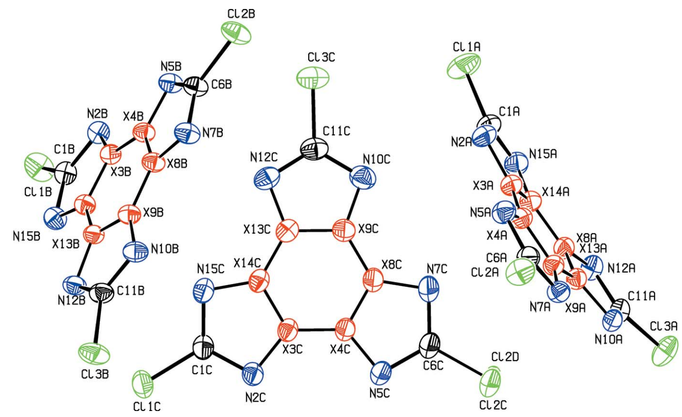


Figure 1
The three independent molecules in the title compound. Displacement ellipsoids are drawn at the 50% probability level. The atoms depicted with *X* are statistically occupied by C and N atoms.

occupation of C and N atoms with the same atomic displacement parameters using EADP and EXYZ instructions (Sheldrick, 2015). Moreover, in molecule C, one of the Cl atoms (Cl2) was refined as disordered over two sets of sites in a ratio of 0.6:0.4.

Acknowledgements

The authors are grateful to Michael Müller for the preparation of the title compound.

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full crystallographic data

IUCrData (2018). **3**, x180212 [https://doi.org/10.1107/S2414314618002122]

2,6,10-Trichlorotris[1,2,4]triazolo[1,5-*a*:1′,5′-*c*:1″,5″-*e*][1,3,5]triazine

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2,6,10-Trichlorotris[1,2,4]triazolo[1,5-*a*:1′,5′-*c*:1″,5″-*e*][1,3,5]triazine

Crystal data

$C_6Cl_3N_9$
M_r = 304.50
Monoclinic, *I*2/*a*
a = 22.2914 (8) Å
b = 14.1339 (3) Å
c = 23.1869 (8) Å
β = 115.732 (2)°
V = 6580.9 (4) Å^3
Z = 24
$F(000)$ = 3600
D_x = 1.844 Mg m^{-3}
Melting point: 587 K
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 23263 reflections
θ = 2.3–28.5°
μ = 0.83 mm^{-1}
T = 193 K
Block, colourless
0.30 × 0.28 × 0.18 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (*X-RED* and *X-Shape*; Stoe, 2006)
T_{min} = 0.769, T_{max} = 0.877
18928 measured reflections
8167 independent reflections
6939 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 28.4°, θ_{min} = 2.3°
$h = -29 \rightarrow 25$
$k = -18 \rightarrow 16$
$l = -30 \rightarrow 30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.086
S = 1.06
8167 reflections
496 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 6.6621P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Cl1A	0.50148 (3)	0.39879 (5)	0.18532 (3)	0.05342 (14)	
Cl2A	0.87848 (2)	0.30279 (4)	0.19801 (2)	0.03969 (11)	
Cl3A	0.53692 (2)	0.14426 (4)	−0.12187 (2)	0.04084 (11)	
C1A	0.55042 (10)	0.36694 (14)	0.14962 (9)	0.0358 (4)	
N2A	0.61701 (8)	0.36660 (11)	0.18167 (7)	0.0351 (3)	
C3A	0.63338 (8)	0.33339 (11)	0.13616 (7)	0.0284 (3)	0.5
N4A	0.69499 (8)	0.31578 (11)	0.13883 (7)	0.0277 (3)	0.5
C8A	0.70030 (7)	0.27587 (10)	0.08791 (7)	0.0256 (3)	0.5
N9A	0.64387 (7)	0.25150 (10)	0.03465 (7)	0.0253 (3)	0.5
C13A	0.58295 (7)	0.27325 (11)	0.03056 (7)	0.0269 (3)	0.5
N14A	0.57768 (8)	0.31568 (11)	0.08143 (7)	0.0282 (3)	0.5
N3A	0.63338 (8)	0.33339 (11)	0.13616 (7)	0.0284 (3)	0.5
C4A	0.69499 (8)	0.31578 (11)	0.13883 (7)	0.0277 (3)	0.5
N8A	0.70030 (7)	0.27587 (10)	0.08791 (7)	0.0256 (3)	0.5
C9A	0.64387 (7)	0.25150 (10)	0.03465 (7)	0.0253 (3)	0.5
N13A	0.58295 (7)	0.27325 (11)	0.03056 (7)	0.0269 (3)	0.5
C14A	0.57768 (8)	0.31568 (11)	0.08143 (7)	0.0282 (3)	0.5
N5A	0.75582 (7)	0.33290 (11)	0.18605 (7)	0.0317 (3)	
C6A	0.79407 (8)	0.29961 (13)	0.15889 (8)	0.0297 (3)	
N7A	0.76412 (7)	0.26461 (10)	0.09948 (7)	0.0283 (3)	
N10A	0.63844 (7)	0.20501 (10)	−0.01787 (6)	0.0267 (3)	
C11A	0.57228 (8)	0.20145 (12)	−0.05080 (8)	0.0286 (3)	
N12A	0.53476 (7)	0.24124 (11)	−0.02468 (7)	0.0310 (3)	
N15A	0.52289 (8)	0.33746 (11)	0.08844 (8)	0.0340 (3)	
Cl1B	−0.03894 (2)	−0.14517 (4)	0.12323 (2)	0.04130 (11)	
Cl2B	0.19373 (2)	0.26427 (3)	0.37720 (2)	0.03809 (11)	
Cl3B	0.34584 (2)	−0.04467 (4)	0.16120 (2)	0.04261 (12)	
C1B	0.03567 (8)	−0.09030 (12)	0.15949 (7)	0.0272 (3)	
N2B	0.04426 (7)	−0.02136 (10)	0.20196 (6)	0.0262 (3)	
C3B	0.10762 (7)	0.00306 (10)	0.21697 (7)	0.0240 (3)	0.5
N4B	0.14546 (7)	0.07184 (11)	0.25812 (7)	0.0245 (3)	0.5
C8B	0.20791 (7)	0.08929 (11)	0.26455 (7)	0.0259 (3)	0.5
N9B	0.23295 (7)	0.03744 (11)	0.22978 (7)	0.0258 (3)	0.5
C13B	0.19638 (7)	−0.03440 (10)	0.19183 (7)	0.0244 (3)	0.5
N14B	0.13290 (7)	−0.05090 (10)	0.18444 (7)	0.0250 (3)	0.5
N3B	0.10762 (7)	0.00306 (10)	0.21697 (7)	0.0240 (3)	0.5
C4B	0.14546 (7)	0.07184 (11)	0.25812 (7)	0.0245 (3)	0.5
N8B	0.20791 (7)	0.08929 (11)	0.26455 (7)	0.0259 (3)	0.5
C9B	0.23295 (7)	0.03744 (11)	0.22978 (7)	0.0258 (3)	0.5
N13B	0.19638 (7)	−0.03440 (10)	0.19183 (7)	0.0244 (3)	0.5
C14B	0.13290 (7)	−0.05090 (10)	0.18444 (7)	0.0250 (3)	0.5
N5B	0.12973 (7)	0.12899 (11)	0.29535 (6)	0.0281 (3)	
C6B	0.18603 (8)	0.17931 (12)	0.32303 (7)	0.0281 (3)	
N7B	0.23611 (7)	0.15932 (11)	0.30712 (7)	0.0300 (3)	
N10B	0.29105 (7)	0.04625 (11)	0.22639 (7)	0.0300 (3)	

C11B	0.28553 (8)	−0.02412 (13)	0.18536 (8)	0.0299 (3)	
N12B	0.22964 (7)	−0.07627 (11)	0.16268 (7)	0.0290 (3)	
N15B	0.08717 (7)	−0.11262 (10)	0.14640 (6)	0.0287 (3)	
Cl1C	0.32389 (3)	0.50215 (3)	0.48481 (2)	0.04398 (12)	
Cl2C	0.37800 (10)	−0.07162 (15)	0.57091 (10)	0.0609 (5)	0.6
Cl2D	0.3429 (2)	−0.0747 (2)	0.55162 (17)	0.0867 (12)	0.4
Cl3C	0.44665 (3)	0.14551 (4)	0.26997 (2)	0.04630 (12)	
C1C	0.33835 (9)	0.39221 (12)	0.46512 (8)	0.0299 (3)	
N2C	0.33716 (7)	0.31761 (10)	0.50027 (6)	0.0294 (3)	
C3C	0.35413 (8)	0.24852 (11)	0.47082 (7)	0.0275 (3)	0.5
N4C	0.36250 (9)	0.15409 (11)	0.48472 (7)	0.0325 (3)	0.5
C8C	0.38457 (10)	0.09598 (11)	0.45145 (8)	0.0363 (4)	0.5
N9C	0.39712 (8)	0.13188 (12)	0.40286 (7)	0.0313 (3)	0.5
C13C	0.38372 (8)	0.22401 (11)	0.38575 (7)	0.0282 (3)	0.5
N14C	0.36346 (8)	0.28308 (11)	0.42062 (7)	0.0274 (3)	0.5
N3C	0.35413 (8)	0.24852 (11)	0.47082 (7)	0.0275 (3)	0.5
C4C	0.36250 (9)	0.15409 (11)	0.48472 (7)	0.0325 (3)	0.5
N8C	0.38457 (10)	0.09598 (11)	0.45145 (8)	0.0363 (4)	0.5
C9C	0.39712 (8)	0.13188 (12)	0.40286 (7)	0.0313 (3)	0.5
N13C	0.38372 (8)	0.22401 (11)	0.38575 (7)	0.0282 (3)	0.5
C14C	0.36346 (8)	0.28308 (11)	0.42062 (7)	0.0274 (3)	0.5
N5C	0.35267 (11)	0.10627 (12)	0.52975 (8)	0.0474 (5)	
C6C	0.37046 (18)	0.01955 (15)	0.51999 (12)	0.0617 (8)	
N7C	0.38969 (13)	0.00700 (12)	0.47299 (9)	0.0554 (5)	
N10C	0.42092 (8)	0.08836 (12)	0.36577 (7)	0.0377 (3)	
C11C	0.41959 (9)	0.16014 (14)	0.32734 (8)	0.0343 (4)	
N12C	0.39729 (7)	0.24434 (11)	0.33634 (7)	0.0319 (3)	
N15C	0.35373 (8)	0.37692 (10)	0.41579 (7)	0.0313 (3)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1A	0.0482 (3)	0.0708 (4)	0.0576 (3)	0.0050 (3)	0.0382 (3)	−0.0124 (3)
Cl2A	0.0262 (2)	0.0532 (3)	0.0350 (2)	−0.00606 (18)	0.00887 (16)	−0.00842 (19)
Cl3A	0.0296 (2)	0.0474 (3)	0.0382 (2)	0.00202 (18)	0.00787 (17)	−0.01813 (19)
C1A	0.0391 (10)	0.0357 (9)	0.0432 (10)	0.0012 (8)	0.0277 (8)	−0.0044 (7)
N2A	0.0407 (8)	0.0368 (8)	0.0365 (8)	−0.0006 (7)	0.0250 (7)	−0.0059 (6)
C3A	0.0313 (8)	0.0273 (7)	0.0316 (7)	−0.0007 (6)	0.0183 (6)	−0.0021 (6)
N4A	0.0289 (7)	0.0287 (7)	0.0278 (7)	−0.0032 (6)	0.0144 (6)	−0.0033 (6)
C8A	0.0258 (7)	0.0264 (7)	0.0262 (6)	−0.0022 (6)	0.0127 (6)	−0.0020 (5)
N9A	0.0252 (7)	0.0241 (7)	0.0278 (7)	−0.0013 (5)	0.0124 (6)	−0.0019 (5)
C13A	0.0272 (7)	0.0253 (7)	0.0297 (7)	0.0009 (6)	0.0138 (6)	−0.0012 (6)
N14A	0.0297 (7)	0.0278 (7)	0.0319 (7)	0.0000 (6)	0.0179 (6)	−0.0008 (6)
N3A	0.0313 (8)	0.0273 (7)	0.0316 (7)	−0.0007 (6)	0.0183 (6)	−0.0021 (6)
C4A	0.0289 (7)	0.0287 (7)	0.0278 (7)	−0.0032 (6)	0.0144 (6)	−0.0033 (6)
N8A	0.0258 (7)	0.0264 (7)	0.0262 (6)	−0.0022 (6)	0.0127 (6)	−0.0020 (5)
C9A	0.0252 (7)	0.0241 (7)	0.0278 (7)	−0.0013 (5)	0.0124 (6)	−0.0019 (5)
N13A	0.0272 (7)	0.0253 (7)	0.0297 (7)	0.0009 (6)	0.0138 (6)	−0.0012 (6)

C14A	0.0297 (7)	0.0278 (7)	0.0319 (7)	0.0000 (6)	0.0179 (6)	−0.0008 (6)
N5A	0.0301 (7)	0.0357 (8)	0.0288 (7)	−0.0060 (6)	0.0124 (6)	−0.0064 (6)
C6A	0.0287 (8)	0.0321 (8)	0.0280 (7)	−0.0040 (7)	0.0120 (6)	−0.0026 (6)
N7A	0.0251 (7)	0.0317 (7)	0.0295 (7)	−0.0033 (6)	0.0131 (5)	−0.0025 (5)
N10A	0.0288 (7)	0.0241 (6)	0.0278 (6)	−0.0002 (5)	0.0128 (5)	−0.0040 (5)
C11A	0.0273 (8)	0.0251 (7)	0.0308 (8)	0.0006 (6)	0.0103 (6)	−0.0045 (6)
N12A	0.0267 (7)	0.0304 (7)	0.0339 (7)	0.0002 (6)	0.0115 (6)	−0.0047 (6)
N15A	0.0320 (7)	0.0335 (8)	0.0442 (8)	−0.0002 (6)	0.0235 (7)	−0.0027 (6)
Cl1B	0.0257 (2)	0.0455 (3)	0.0466 (2)	−0.00941 (18)	0.00993 (18)	−0.0154 (2)
Cl2B	0.0333 (2)	0.0451 (2)	0.0369 (2)	−0.00612 (18)	0.01624 (17)	−0.01918 (18)
Cl3B	0.0353 (2)	0.0547 (3)	0.0499 (3)	0.0018 (2)	0.0298 (2)	−0.0085 (2)
C1B	0.0229 (7)	0.0290 (8)	0.0256 (7)	−0.0008 (6)	0.0066 (6)	0.0004 (6)
N2B	0.0205 (6)	0.0289 (7)	0.0270 (6)	0.0005 (5)	0.0083 (5)	0.0010 (5)
C3B	0.0223 (6)	0.0260 (7)	0.0237 (6)	−0.0001 (5)	0.0100 (5)	−0.0002 (5)
N4B	0.0219 (6)	0.0281 (7)	0.0251 (6)	−0.0022 (5)	0.0117 (5)	−0.0029 (5)
C8B	0.0226 (7)	0.0305 (7)	0.0263 (6)	−0.0017 (6)	0.0124 (5)	−0.0037 (5)
N9B	0.0237 (7)	0.0303 (7)	0.0250 (6)	0.0005 (6)	0.0122 (5)	−0.0008 (5)
C13B	0.0258 (7)	0.0259 (7)	0.0239 (6)	0.0024 (5)	0.0131 (5)	0.0004 (5)
N14B	0.0244 (7)	0.0262 (7)	0.0245 (6)	0.0008 (6)	0.0108 (5)	−0.0003 (5)
N3B	0.0223 (6)	0.0260 (7)	0.0237 (6)	−0.0001 (5)	0.0100 (5)	−0.0002 (5)
C4B	0.0219 (6)	0.0281 (7)	0.0251 (6)	−0.0022 (5)	0.0117 (5)	−0.0029 (5)
N8B	0.0226 (7)	0.0305 (7)	0.0263 (6)	−0.0017 (6)	0.0124 (5)	−0.0037 (5)
C9B	0.0237 (7)	0.0303 (7)	0.0250 (6)	0.0005 (6)	0.0122 (5)	−0.0008 (5)
N13B	0.0258 (7)	0.0259 (7)	0.0239 (6)	0.0024 (5)	0.0131 (5)	0.0004 (5)
C14B	0.0244 (7)	0.0262 (7)	0.0245 (6)	0.0008 (6)	0.0108 (5)	−0.0003 (5)
N5B	0.0266 (7)	0.0332 (7)	0.0277 (6)	−0.0023 (6)	0.0147 (5)	−0.0056 (5)
C6B	0.0260 (7)	0.0340 (8)	0.0252 (7)	−0.0024 (6)	0.0119 (6)	−0.0062 (6)
N7B	0.0251 (7)	0.0361 (8)	0.0290 (7)	−0.0053 (6)	0.0120 (5)	−0.0088 (6)
N10B	0.0243 (7)	0.0374 (8)	0.0324 (7)	0.0011 (6)	0.0161 (6)	−0.0011 (6)
C11B	0.0269 (8)	0.0370 (9)	0.0296 (8)	0.0053 (7)	0.0159 (6)	0.0020 (6)
N12B	0.0308 (7)	0.0329 (7)	0.0277 (6)	0.0049 (6)	0.0167 (6)	−0.0004 (5)
N15B	0.0277 (7)	0.0297 (7)	0.0259 (6)	−0.0018 (6)	0.0089 (5)	−0.0034 (5)
Cl1C	0.0671 (3)	0.0253 (2)	0.0365 (2)	0.0053 (2)	0.0195 (2)	0.00042 (16)
Cl2C	0.1152 (13)	0.0258 (5)	0.0583 (9)	0.0025 (8)	0.0531 (9)	0.0101 (5)
Cl2D	0.190 (4)	0.0261 (8)	0.088 (2)	−0.001 (2)	0.101 (3)	0.0078 (13)
Cl3C	0.0477 (3)	0.0601 (3)	0.0392 (2)	−0.0060 (2)	0.0265 (2)	−0.0083 (2)
C1C	0.0332 (8)	0.0255 (8)	0.0242 (7)	−0.0017 (6)	0.0061 (6)	0.0002 (6)
N2C	0.0347 (7)	0.0251 (7)	0.0238 (6)	−0.0039 (6)	0.0085 (5)	−0.0030 (5)
C3C	0.0316 (7)	0.0240 (7)	0.0231 (6)	−0.0040 (6)	0.0081 (6)	−0.0001 (5)
N4C	0.0472 (9)	0.0236 (7)	0.0275 (7)	−0.0015 (7)	0.0170 (7)	0.0011 (6)
C8C	0.0551 (11)	0.0244 (7)	0.0308 (8)	0.0008 (7)	0.0198 (7)	0.0016 (6)
N9C	0.0364 (8)	0.0303 (8)	0.0259 (7)	−0.0005 (6)	0.0123 (6)	−0.0015 (6)
C13C	0.0256 (7)	0.0309 (8)	0.0255 (7)	−0.0036 (6)	0.0085 (6)	0.0010 (6)
N14C	0.0281 (7)	0.0257 (7)	0.0247 (6)	−0.0022 (6)	0.0081 (6)	0.0026 (5)
N3C	0.0316 (7)	0.0240 (7)	0.0231 (6)	−0.0040 (6)	0.0081 (6)	−0.0001 (5)
C4C	0.0472 (9)	0.0236 (7)	0.0275 (7)	−0.0015 (7)	0.0170 (7)	0.0011 (6)
N8C	0.0551 (11)	0.0244 (7)	0.0308 (8)	0.0008 (7)	0.0198 (7)	0.0016 (6)
C9C	0.0364 (8)	0.0303 (8)	0.0259 (7)	−0.0005 (6)	0.0123 (6)	−0.0015 (6)

N13C	0.0256 (7)	0.0309 (8)	0.0255 (7)	−0.0036 (6)	0.0085 (6)	0.0010 (6)
C14C	0.0281 (7)	0.0257 (7)	0.0247 (6)	−0.0022 (6)	0.0081 (6)	0.0026 (5)
N5C	0.0880 (14)	0.0256 (7)	0.0402 (9)	−0.0033 (8)	0.0387 (9)	0.0018 (6)
C6C	0.126 (2)	0.0252 (9)	0.0548 (13)	−0.0025 (12)	0.0585 (16)	0.0027 (9)
N7C	0.1067 (18)	0.0243 (8)	0.0482 (10)	0.0027 (9)	0.0458 (11)	0.0021 (7)
N10C	0.0422 (9)	0.0388 (8)	0.0315 (7)	0.0011 (7)	0.0156 (7)	−0.0051 (6)
C11C	0.0305 (8)	0.0443 (10)	0.0279 (8)	−0.0067 (7)	0.0124 (7)	−0.0055 (7)
N12C	0.0282 (7)	0.0396 (8)	0.0273 (7)	−0.0070 (6)	0.0114 (6)	0.0003 (6)
N15C	0.0350 (8)	0.0264 (7)	0.0289 (7)	−0.0021 (6)	0.0103 (6)	0.0031 (5)

Geometric parameters (Å, º)

Cl1A—C1A	1.6917 (17)	N14B—N15B	1.341 (2)
Cl2A—C6A	1.6980 (17)	N3B—C14B	1.355 (2)
Cl3A—C11A	1.6920 (16)	N3B—C4B	1.367 (2)
C1A—N2A	1.341 (3)	C4B—N5B	1.3356 (19)
C1A—N15A	1.344 (2)	C4B—N8B	1.3567 (19)
N2A—N3A	1.342 (2)	N8B—N7B	1.345 (2)
N2A—C3A	1.342 (2)	N8B—C9B	1.3745 (19)
C3A—N14A	1.359 (2)	C9B—N10B	1.3370 (19)
C3A—N4A	1.370 (2)	C9B—N13B	1.359 (2)
N4A—N5A	1.344 (2)	N13B—N12B	1.3385 (19)
N4A—C8A	1.3593 (19)	N13B—C14B	1.370 (2)
C8A—N7A	1.338 (2)	C14B—N15B	1.341 (2)
C8A—N9A	1.370 (2)	N5B—C6B	1.339 (2)
N9A—N10A	1.3423 (19)	C6B—N7B	1.349 (2)
N9A—C13A	1.355 (2)	N10B—C11B	1.345 (2)
C13A—N12A	1.343 (2)	C11B—N12B	1.343 (2)
C13A—N14A	1.373 (2)	Cl1C—C1C	1.6896 (18)
N14A—N15A	1.336 (2)	Cl2C—C6C	1.706 (3)
N3A—C14A	1.359 (2)	Cl2D—C6C	1.756 (4)
N3A—C4A	1.370 (2)	Cl3C—C11C	1.6950 (18)
C4A—N5A	1.344 (2)	C1C—N2C	1.340 (2)
C4A—N8A	1.3593 (19)	C1C—N15C	1.347 (2)
N8A—N7A	1.338 (2)	N2C—N3C	1.337 (2)
N8A—C9A	1.370 (2)	N2C—C3C	1.337 (2)
C9A—N10A	1.3423 (19)	C3C—N14C	1.359 (2)
C9A—N13A	1.355 (2)	C3C—N4C	1.367 (2)
N13A—N12A	1.343 (2)	N4C—N5C	1.339 (2)
N13A—C14A	1.373 (2)	N4C—C8C	1.357 (2)
C14A—N15A	1.336 (2)	C8C—N7C	1.340 (2)
N5A—C6A	1.346 (2)	C8C—N9C	1.371 (2)
C6A—N7A	1.338 (2)	N9C—N10C	1.340 (2)
N10A—C11A	1.335 (2)	N9C—C13C	1.356 (2)
C11A—N12A	1.350 (2)	C13C—N12C	1.337 (2)
Cl1B—C1B	1.6913 (17)	C13C—N14C	1.368 (2)
Cl2B—C6B	1.6917 (16)	N14C—N15C	1.341 (2)
Cl3B—C11B	1.6908 (16)	N3C—C14C	1.359 (2)

C1B—N2B	1.339 (2)	N3C—C4C	1.367 (2)
C1B—N15B	1.346 (2)	C4C—N5C	1.339 (2)
N2B—N3B	1.3446 (19)	C4C—N8C	1.357 (2)
N2B—C3B	1.3446 (19)	N8C—N7C	1.340 (2)
C3B—N14B	1.355 (2)	N8C—C9C	1.371 (2)
C3B—N4B	1.367 (2)	C9C—N10C	1.340 (2)
N4B—N5B	1.3356 (19)	C9C—N13C	1.356 (2)
N4B—C8B	1.3567 (19)	N13C—N12C	1.337 (2)
C8B—N7B	1.345 (2)	N13C—C14C	1.368 (2)
C8B—N9B	1.3745 (19)	C14C—N15C	1.341 (2)
N9B—N10B	1.3370 (19)	N5C—C6C	1.337 (3)
N9B—C13B	1.359 (2)	C6C—N7C	1.345 (3)
C13B—N12B	1.3385 (19)	N10C—C11C	1.342 (3)
C13B—N14B	1.370 (2)	C11C—N12C	1.340 (2)

N2A—C1A—N15A	118.16 (15)	N7B—N8B—C9B	130.03 (14)
N2A—C1A—Cl1A	121.58 (14)	C4B—N8B—C9B	119.81 (14)
N15A—C1A—Cl1A	120.20 (15)	N10B—C9B—N13B	110.82 (13)
C1A—N2A—N3A	100.32 (14)	N10B—C9B—N8B	129.44 (15)
C1A—N2A—C3A	100.32 (14)	N13B—C9B—N8B	119.74 (13)
N2A—C3A—N14A	110.39 (14)	N12B—N13B—C9B	110.44 (13)
N2A—C3A—N4A	129.58 (15)	N12B—N13B—C14B	129.07 (14)
N14A—C3A—N4A	120.02 (14)	C9B—N13B—C14B	120.32 (13)
N5A—N4A—C8A	110.17 (14)	N15B—C14B—N3B	110.56 (13)
N5A—N4A—C3A	129.86 (14)	N15B—C14B—N13B	129.96 (14)
C8A—N4A—C3A	119.97 (14)	N3B—C14B—N13B	119.42 (14)
N7A—C8A—N4A	111.18 (13)	C4B—N5B—C6B	100.17 (13)
N7A—C8A—N9A	129.13 (14)	N4B—N5B—C6B	100.17 (13)
N4A—C8A—N9A	119.68 (14)	N5B—C6B—N7B	118.18 (14)
N10A—N9A—C13A	110.78 (13)	N5B—C6B—Cl2B	120.31 (12)
N10A—N9A—C8A	128.80 (14)	N7B—C6B—Cl2B	121.50 (13)
C13A—N9A—C8A	120.41 (14)	N8B—N7B—C6B	100.15 (13)
N12A—C13A—N9A	110.64 (13)	C8B—N7B—C6B	100.15 (13)
N12A—C13A—N14A	129.42 (15)	C9B—N10B—C11B	100.34 (14)
N9A—C13A—N14A	119.74 (14)	N9B—N10B—C11B	100.34 (14)
N15A—N14A—C3A	110.91 (14)	N12B—C11B—N10B	117.86 (14)
N15A—N14A—C13A	128.97 (15)	N12B—C11B—Cl3B	120.79 (13)
C3A—N14A—C13A	119.89 (14)	N10B—C11B—Cl3B	121.32 (14)
N2A—N3A—C14A	110.39 (14)	N13B—N12B—C11B	100.53 (13)
N2A—N3A—C4A	129.58 (15)	C13B—N12B—C11B	100.53 (13)
C14A—N3A—C4A	120.02 (14)	C14B—N15B—C1B	100.28 (13)
N5A—C4A—N8A	110.17 (14)	N14B—N15B—C1B	100.28 (13)
N5A—C4A—N3A	129.86 (14)	N2C—C1C—N15C	118.03 (15)
N8A—C4A—N3A	119.97 (14)	N2C—C1C—Cl1C	120.19 (13)
N7A—N8A—C4A	111.18 (13)	N15C—C1C—Cl1C	121.73 (13)
N7A—N8A—C9A	129.13 (14)	N3C—N2C—C1C	100.34 (13)
C4A—N8A—C9A	119.68 (14)	C3C—N2C—C1C	100.34 (13)
N10A—C9A—N13A	110.78 (13)	N2C—C3C—N14C	110.94 (14)

N10A—C9A—N8A	128.80 (14)	N2C—C3C—N4C	129.26 (15)
N13A—C9A—N8A	120.41 (14)	N14C—C3C—N4C	119.80 (15)
N12A—N13A—C9A	110.64 (13)	N5C—N4C—C8C	111.11 (15)
N12A—N13A—C14A	129.42 (15)	N5C—N4C—C3C	128.67 (16)
C9A—N13A—C14A	119.74 (14)	C8C—N4C—C3C	120.21 (15)
N15A—C14A—N3A	110.91 (14)	N7C—C8C—N4C	110.46 (16)
N15A—C14A—N13A	128.97 (15)	N7C—C8C—N9C	129.73 (17)
N3A—C14A—N13A	119.89 (14)	N4C—C8C—N9C	119.80 (15)
C4A—N5A—C6A	100.13 (13)	N10C—N9C—C13C	110.55 (15)
N4A—N5A—C6A	100.13 (13)	N10C—N9C—C8C	129.54 (16)
N7A—C6A—N5A	118.49 (15)	C13C—N9C—C8C	119.89 (15)
N7A—C6A—Cl2A	120.11 (13)	N12C—C13C—N9C	110.74 (15)
N5A—C6A—Cl2A	121.40 (13)	N12C—C13C—N14C	129.10 (15)
C6A—N7A—C8A	100.03 (13)	N9C—C13C—N14C	120.02 (14)
C6A—N7A—N8A	100.03 (13)	N15C—N14C—C3C	110.34 (14)
C11A—N10A—N9A	100.33 (13)	N15C—N14C—C13C	129.60 (14)
C11A—N10A—C9A	100.33 (13)	C3C—N14C—C13C	119.95 (14)
N10A—C11A—N12A	118.26 (14)	N2C—N3C—C14C	110.94 (14)
N10A—C11A—Cl3A	120.44 (12)	N2C—N3C—C4C	129.26 (15)
N12A—C11A—Cl3A	121.25 (13)	C14C—N3C—C4C	119.80 (15)
N13A—N12A—C11A	99.99 (13)	N5C—C4C—N8C	111.11 (15)
C13A—N12A—C11A	99.99 (13)	N5C—C4C—N3C	128.67 (16)
C14A—N15A—C1A	100.21 (15)	N8C—C4C—N3C	120.21 (15)
N14A—N15A—C1A	100.21 (15)	N7C—N8C—C4C	110.46 (16)
N2B—C1B—N15B	118.21 (14)	N7C—N8C—C9C	129.73 (17)
N2B—C1B—Cl1B	119.68 (13)	C4C—N8C—C9C	119.80 (15)
N15B—C1B—Cl1B	122.10 (13)	N10C—C9C—N13C	110.55 (15)
C1B—N2B—N3B	100.14 (13)	N10C—C9C—N8C	129.54 (16)
C1B—N2B—C3B	100.14 (13)	N13C—C9C—N8C	119.89 (15)
N2B—C3B—N14B	110.81 (13)	N12C—N13C—C9C	110.74 (15)
N2B—C3B—N4B	128.60 (14)	N12C—N13C—C14C	129.10 (15)
N14B—C3B—N4B	120.59 (13)	C9C—N13C—C14C	120.02 (14)
N5B—N4B—C8B	111.34 (13)	N15C—C14C—N3C	110.34 (14)
N5B—N4B—C3B	128.73 (14)	N15C—C14C—N13C	129.60 (14)
C8B—N4B—C3B	119.93 (13)	N3C—C14C—N13C	119.95 (14)
N7B—C8B—N4B	110.16 (13)	C6C—N5C—N4C	99.77 (16)
N7B—C8B—N9B	130.03 (14)	C6C—N5C—C4C	99.77 (16)
N4B—C8B—N9B	119.81 (14)	N5C—C6C—N7C	118.70 (18)
N10B—N9B—C13B	110.82 (13)	N5C—C6C—Cl2C	121.50 (18)
N10B—N9B—C8B	129.44 (15)	N7C—C6C—Cl2C	119.40 (19)
C13B—N9B—C8B	119.74 (13)	N5C—C6C—Cl2D	116.2 (2)
N12B—C13B—N9B	110.44 (13)	N7C—C6C—Cl2D	122.1 (2)
N12B—C13B—N14B	129.07 (14)	N8C—N7C—C6C	99.94 (17)
N9B—C13B—N14B	120.32 (13)	C8C—N7C—C6C	99.94 (17)
N15B—N14B—C3B	110.56 (13)	C9C—N10C—C11C	100.27 (15)
N15B—N14B—C13B	129.96 (14)	N9C—N10C—C11C	100.27 (15)
C3B—N14B—C13B	119.42 (14)	N12C—C11C—N10C	118.08 (16)
N2B—N3B—C14B	110.81 (13)	N12C—C11C—Cl3C	120.85 (14)

N2B—N3B—C4B	128.60 (14)	N10C—C11C—Cl3C	121.06 (15)
C14B—N3B—C4B	120.59 (13)	N13C—N12C—C11C	100.35 (14)
N5B—C4B—N8B	111.34 (13)	C13C—N12C—C11C	100.35 (14)
N5B—C4B—N3B	128.73 (14)	C14C—N15C—C1C	100.34 (13)
N8B—C4B—N3B	119.93 (13)	N14C—N15C—C1C	100.34 (13)
N7B—N8B—C4B	110.16 (13)		

N15A—C1A—N2A—N3A	−0.1 (2)	N2B—N3B—C14B—N15B	0.38 (18)
Cl1A—C1A—N2A—N3A	177.29 (14)	C4B—N3B—C14B—N15B	−179.17 (14)
N15A—C1A—N2A—C3A	−0.1 (2)	N2B—N3B—C14B—N13B	177.88 (13)
Cl1A—C1A—N2A—C3A	177.29 (14)	C4B—N3B—C14B—N13B	−1.7 (2)
C1A—N2A—C3A—N14A	−0.39 (19)	N12B—N13B—C14B—N15B	−0.1 (3)
C1A—N2A—C3A—N4A	−179.60 (18)	C9B—N13B—C14B—N15B	174.78 (15)
N2A—C3A—N4A—N5A	−5.1 (3)	N12B—N13B—C14B—N3B	−177.05 (15)
N14A—C3A—N4A—N5A	175.73 (17)	C9B—N13B—C14B—N3B	−2.2 (2)
N2A—C3A—N4A—C8A	175.62 (16)	N8B—C4B—N5B—C6B	−0.03 (18)
N14A—C3A—N4A—C8A	−3.5 (2)	N3B—C4B—N5B—C6B	−179.63 (16)
N5A—N4A—C8A—N7A	0.39 (19)	C8B—N4B—N5B—C6B	−0.03 (18)
C3A—N4A—C8A—N7A	179.78 (14)	C3B—N4B—N5B—C6B	−179.63 (16)
N5A—N4A—C8A—N9A	179.14 (14)	C4B—N5B—C6B—N7B	−0.3 (2)
C3A—N4A—C8A—N9A	−1.5 (2)	N4B—N5B—C6B—N7B	−0.3 (2)
N7A—C8A—N9A—N10A	4.4 (3)	C4B—N5B—C6B—Cl2B	−179.36 (13)
N4A—C8A—N9A—N10A	−174.10 (15)	N4B—N5B—C6B—Cl2B	−179.36 (13)
N7A—C8A—N9A—C13A	−176.60 (16)	C4B—N8B—N7B—C6B	−0.40 (18)
N4A—C8A—N9A—C13A	4.9 (2)	C9B—N8B—N7B—C6B	179.77 (17)
N10A—N9A—C13A—N12A	0.52 (19)	N4B—C8B—N7B—C6B	−0.40 (18)
C8A—N9A—C13A—N12A	−178.64 (14)	N9B—C8B—N7B—C6B	179.77 (17)
N10A—N9A—C13A—N14A	175.86 (14)	N5B—C6B—N7B—N8B	0.4 (2)
C8A—N9A—C13A—N14A	−3.3 (2)	Cl2B—C6B—N7B—N8B	179.52 (13)
N2A—C3A—N14A—N15A	0.8 (2)	N5B—C6B—N7B—C8B	0.4 (2)
N4A—C3A—N14A—N15A	−179.95 (15)	Cl2B—C6B—N7B—C8B	179.52 (13)
N2A—C3A—N14A—C13A	−174.17 (15)	N13B—C9B—N10B—C11B	−0.45 (18)
N4A—C3A—N14A—C13A	5.1 (2)	N8B—C9B—N10B—C11B	179.83 (16)
N12A—C13A—N14A—N15A	−1.3 (3)	C13B—N9B—N10B—C11B	−0.45 (18)
N9A—C13A—N14A—N15A	−175.61 (16)	C8B—N9B—N10B—C11B	179.83 (16)
N12A—C13A—N14A—C3A	172.63 (16)	C9B—N10B—C11B—N12B	0.0 (2)
N9A—C13A—N14A—C3A	−1.7 (2)	N9B—N10B—C11B—N12B	0.0 (2)
C1A—N2A—N3A—C14A	−0.39 (19)	C9B—N10B—C11B—Cl3B	178.23 (12)
C1A—N2A—N3A—C4A	−179.60 (18)	N9B—N10B—C11B—Cl3B	178.23 (12)
N2A—N3A—C4A—N5A	−5.1 (3)	C9B—N13B—N12B—C11B	−0.72 (17)
C14A—N3A—C4A—N5A	175.73 (17)	C14B—N13B—N12B—C11B	174.57 (16)
N2A—N3A—C4A—N8A	175.62 (16)	N9B—C13B—N12B—C11B	−0.72 (17)
C14A—N3A—C4A—N8A	−3.5 (2)	N14B—C13B—N12B—C11B	174.57 (16)
N5A—C4A—N8A—N7A	0.39 (19)	N10B—C11B—N12B—N13B	0.5 (2)
N3A—C4A—N8A—N7A	179.78 (14)	Cl3B—C11B—N12B—N13B	−177.80 (12)
N5A—C4A—N8A—C9A	179.14 (14)	N10B—C11B—N12B—C13B	0.5 (2)
N3A—C4A—N8A—C9A	−1.5 (2)	Cl3B—C11B—N12B—C13B	−177.80 (12)
N7A—N8A—C9A—N10A	4.4 (3)	N3B—C14B—N15B—C1B	−0.06 (17)

C4A—N8A—C9A—N10A	−174.10 (15)	N13B—C14B—N15B—C1B	−177.21 (16)
N7A—N8A—C9A—N13A	−176.60 (16)	C3B—N14B—N15B—C1B	−0.06 (17)
C4A—N8A—C9A—N13A	4.9 (2)	C13B—N14B—N15B—C1B	−177.21 (16)
N10A—C9A—N13A—N12A	0.52 (19)	N2B—C1B—N15B—C14B	−0.30 (19)
N8A—C9A—N13A—N12A	−178.64 (14)	Cl1B—C1B—N15B—C14B	178.69 (12)
N10A—C9A—N13A—C14A	175.86 (14)	N2B—C1B—N15B—N14B	−0.30 (19)
N8A—C9A—N13A—C14A	−3.3 (2)	Cl1B—C1B—N15B—N14B	178.69 (12)
N2A—N3A—C14A—N15A	0.8 (2)	N15C—C1C—N2C—N3C	0.7 (2)
C4A—N3A—C14A—N15A	−179.95 (15)	Cl1C—C1C—N2C—N3C	−176.86 (13)
N2A—N3A—C14A—N13A	−174.17 (15)	N15C—C1C—N2C—C3C	0.7 (2)
C4A—N3A—C14A—N13A	5.1 (2)	Cl1C—C1C—N2C—C3C	−176.86 (13)
N12A—N13A—C14A—N15A	−1.3 (3)	C1C—N2C—C3C—N14C	−0.86 (17)
C9A—N13A—C14A—N15A	−175.61 (16)	C1C—N2C—C3C—N4C	179.11 (18)
N12A—N13A—C14A—N3A	172.63 (16)	N2C—C3C—N4C—N5C	3.5 (3)
C9A—N13A—C14A—N3A	−1.7 (2)	N14C—C3C—N4C—N5C	−176.54 (19)
N8A—C4A—N5A—C6A	−0.72 (18)	N2C—C3C—N4C—C8C	−175.34 (17)
N3A—C4A—N5A—C6A	179.97 (17)	N14C—C3C—N4C—C8C	4.6 (3)
C8A—N4A—N5A—C6A	−0.72 (18)	N5C—N4C—C8C—N7C	0.5 (3)
C3A—N4A—N5A—C6A	179.97 (17)	C3C—N4C—C8C—N7C	179.51 (19)
C4A—N5A—C6A—N7A	0.9 (2)	N5C—N4C—C8C—N9C	179.58 (18)
N4A—N5A—C6A—N7A	0.9 (2)	C3C—N4C—C8C—N9C	−1.4 (3)
C4A—N5A—C6A—Cl2A	−179.94 (13)	N7C—C8C—N9C—N10C	−3.5 (4)
N4A—N5A—C6A—Cl2A	−179.94 (13)	N4C—C8C—N9C—N10C	177.59 (18)
N5A—C6A—N7A—C8A	−0.7 (2)	N7C—C8C—N9C—C13C	175.0 (2)
Cl2A—C6A—N7A—C8A	−179.85 (13)	N4C—C8C—N9C—C13C	−3.9 (3)
N5A—C6A—N7A—N8A	−0.7 (2)	N10C—N9C—C13C—N12C	0.8 (2)
Cl2A—C6A—N7A—N8A	−179.85 (13)	C8C—N9C—C13C—N12C	−177.96 (16)
N4A—C8A—N7A—C6A	0.15 (18)	N10C—N9C—C13C—N14C	−175.27 (15)
N9A—C8A—N7A—C6A	−178.46 (17)	C8C—N9C—C13C—N14C	5.9 (2)
C4A—N8A—N7A—C6A	0.15 (18)	N2C—C3C—N14C—N15C	0.81 (19)
C9A—N8A—N7A—C6A	−178.46 (17)	N4C—C3C—N14C—N15C	−179.17 (15)
C13A—N9A—N10A—C11A	−0.39 (17)	N2C—C3C—N14C—C13C	177.41 (14)
C8A—N9A—N10A—C11A	178.68 (16)	N4C—C3C—N14C—C13C	−2.6 (2)
N13A—C9A—N10A—C11A	−0.39 (17)	N12C—C13C—N14C—N15C	−2.1 (3)
N8A—C9A—N10A—C11A	178.68 (16)	N9C—C13C—N14C—N15C	173.15 (16)
N9A—N10A—C11A—N12A	0.2 (2)	N12C—C13C—N14C—C3C	−178.01 (16)
C9A—N10A—C11A—N12A	0.2 (2)	N9C—C13C—N14C—C3C	−2.7 (2)
N9A—N10A—C11A—Cl3A	−177.25 (12)	C1C—N2C—N3C—C14C	−0.86 (17)
C9A—N10A—C11A—Cl3A	−177.25 (12)	C1C—N2C—N3C—C4C	179.11 (18)
C9A—N13A—N12A—C11A	−0.38 (18)	N2C—N3C—C4C—N5C	3.5 (3)
C14A—N13A—N12A—C11A	−175.13 (17)	C14C—N3C—C4C—N5C	−176.54 (19)
N9A—C13A—N12A—C11A	−0.38 (18)	N2C—N3C—C4C—N8C	−175.34 (17)
N14A—C13A—N12A—C11A	−175.13 (17)	C14C—N3C—C4C—N8C	4.6 (3)
N10A—C11A—N12A—N13A	0.1 (2)	N5C—C4C—N8C—N7C	0.5 (3)
Cl3A—C11A—N12A—N13A	177.51 (13)	N3C—C4C—N8C—N7C	179.51 (19)
N10A—C11A—N12A—C13A	0.1 (2)	N5C—C4C—N8C—C9C	179.58 (18)
Cl3A—C11A—N12A—C13A	177.51 (13)	N3C—C4C—N8C—C9C	−1.4 (3)
N3A—C14A—N15A—C1A	−0.72 (19)	N7C—N8C—C9C—N10C	−3.5 (4)

N13A—C14A—N15A—C1A	173.62 (17)	C4C—N8C—C9C—N10C	177.59 (18)
C3A—N14A—N15A—C1A	−0.72 (19)	N7C—N8C—C9C—N13C	175.0 (2)
C13A—N14A—N15A—C1A	173.62 (17)	C4C—N8C—C9C—N13C	−3.9 (3)
N2A—C1A—N15A—C14A	0.5 (2)	N10C—C9C—N13C—N12C	0.8 (2)
Cl1A—C1A—N15A—C14A	−176.90 (14)	N8C—C9C—N13C—N12C	−177.96 (16)
N2A—C1A—N15A—N14A	0.5 (2)	N10C—C9C—N13C—C14C	−175.27 (15)
Cl1A—C1A—N15A—N14A	−176.90 (14)	N8C—C9C—N13C—C14C	5.9 (2)
N15B—C1B—N2B—N3B	0.52 (19)	N2C—N3C—C14C—N15C	0.81 (19)
Cl1B—C1B—N2B—N3B	−178.50 (12)	C4C—N3C—C14C—N15C	−179.17 (15)
N15B—C1B—N2B—C3B	0.52 (19)	N2C—N3C—C14C—N13C	177.41 (14)
Cl1B—C1B—N2B—C3B	−178.50 (12)	C4C—N3C—C14C—N13C	−2.6 (2)
C1B—N2B—C3B—N14B	−0.51 (17)	N12C—N13C—C14C—N15C	−2.1 (3)
C1B—N2B—C3B—N4B	179.00 (16)	C9C—N13C—C14C—N15C	173.15 (16)
N2B—C3B—N4B—N5B	3.0 (3)	N12C—N13C—C14C—N3C	−178.01 (16)
N14B—C3B—N4B—N5B	−177.58 (15)	C9C—N13C—C14C—N3C	−2.7 (2)
N2B—C3B—N4B—C8B	−176.60 (15)	C8C—N4C—N5C—C6C	0.2 (3)
N14B—C3B—N4B—C8B	2.9 (2)	C3C—N4C—N5C—C6C	−178.7 (2)
N5B—N4B—C8B—N7B	0.29 (19)	N8C—C4C—N5C—C6C	0.2 (3)
C3B—N4B—C8B—N7B	179.93 (14)	N3C—C4C—N5C—C6C	−178.7 (2)
N5B—N4B—C8B—N9B	−179.85 (14)	N4C—N5C—C6C—N7C	−0.9 (3)
C3B—N4B—C8B—N9B	−0.2 (2)	C4C—N5C—C6C—N7C	−0.9 (3)
N7B—C8B—N9B—N10B	−4.1 (3)	N4C—N5C—C6C—Cl2C	171.8 (2)
N4B—C8B—N9B—N10B	176.12 (16)	C4C—N5C—C6C—Cl2D	−161.6 (2)
N7B—C8B—N9B—C13B	176.25 (16)	C4C—N8C—N7C—C6C	−0.9 (3)
N4B—C8B—N9B—C13B	−3.6 (2)	C9C—N8C—N7C—C6C	−179.9 (2)
N10B—N9B—C13B—N12B	0.80 (19)	N4C—C8C—N7C—C6C	−0.9 (3)
C8B—N9B—C13B—N12B	−179.46 (14)	N9C—C8C—N7C—C6C	−179.9 (2)
N10B—N9B—C13B—N14B	−174.97 (14)	N5C—C6C—N7C—N8C	1.1 (4)
C8B—N9B—C13B—N14B	4.8 (2)	Cl2D—C6C—N7C—N8C	160.7 (3)
N2B—C3B—N14B—N15B	0.38 (18)	N5C—C6C—N7C—C8C	1.1 (4)
N4B—C3B—N14B—N15B	−179.17 (14)	Cl2C—C6C—N7C—C8C	−171.7 (2)
N2B—C3B—N14B—C13B	177.88 (13)	N13C—C9C—N10C—C11C	−0.41 (19)
N4B—C3B—N14B—C13B	−1.7 (2)	N8C—C9C—N10C—C11C	178.23 (19)
N12B—C13B—N14B—N15B	−0.1 (3)	C13C—N9C—N10C—C11C	−0.41 (19)
N9B—C13B—N14B—N15B	174.78 (15)	C8C—N9C—N10C—C11C	178.23 (19)
N12B—C13B—N14B—C3B	−177.05 (15)	C9C—N10C—C11C—N12C	−0.1 (2)
N9B—C13B—N14B—C3B	−2.2 (2)	N9C—N10C—C11C—N12C	−0.1 (2)
C1B—N2B—N3B—C14B	−0.51 (17)	C9C—N10C—C11C—Cl3C	178.75 (13)
C1B—N2B—N3B—C4B	179.00 (16)	N9C—N10C—C11C—Cl3C	178.75 (13)
N2B—N3B—C4B—N5B	3.0 (3)	C9C—N13C—N12C—C11C	−0.80 (18)
C14B—N3B—C4B—N5B	−177.58 (15)	C14C—N13C—N12C—C11C	174.84 (17)
N2B—N3B—C4B—N8B	−176.60 (15)	N9C—C13C—N12C—C11C	−0.80 (18)
C14B—N3B—C4B—N8B	2.9 (2)	N14C—C13C—N12C—C11C	174.84 (17)
N5B—C4B—N8B—N7B	0.29 (19)	N10C—C11C—N12C—N13C	0.6 (2)
N3B—C4B—N8B—N7B	179.93 (14)	Cl3C—C11C—N12C—N13C	−178.29 (13)
N5B—C4B—N8B—C9B	−179.85 (14)	N10C—C11C—N12C—C13C	0.6 (2)
N3B—C4B—N8B—C9B	−0.2 (2)	Cl3C—C11C—N12C—C13C	−178.29 (13)
N7B—N8B—C9B—N10B	−4.1 (3)	N3C—C14C—N15C—C1C	−0.33 (18)

C4B—N8B—C9B—N10B	176.12 (16)	N13C—C14C—N15C—C1C	−176.50 (17)
N7B—N8B—C9B—N13B	176.25 (16)	C3C—N14C—N15C—C1C	−0.33 (18)
C4B—N8B—C9B—N13B	−3.6 (2)	C13C—N14C—N15C—C1C	−176.50 (17)
N10B—C9B—N13B—N12B	0.80 (19)	N2C—C1C—N15C—C14C	−0.3 (2)
N8B—C9B—N13B—N12B	−179.46 (14)	Cl1C—C1C—N15C—C14C	177.27 (13)
N10B—C9B—N13B—C14B	−174.97 (14)	N2C—C1C—N15C—N14C	−0.3 (2)
N8B—C9B—N13B—C14B	4.8 (2)	Cl1C—C1C—N15C—N14C	177.27 (13)