

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## 2-(4-Fluorophenyl)-1,4,5-triphenyl-1H-imidazole

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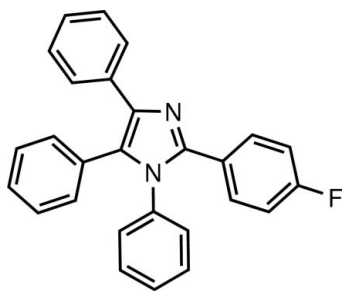
Received 26 August 2010; accepted 2 September 2010

Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.049;  $wR$  factor = 0.128; data-to-parameter ratio = 30.8.

In the title molecule,  $\text{C}_{27}\text{H}_{19}\text{FN}_2$ , the imidazole ring is essentially planar [maximum deviation = 0.004 (1) Å] and makes dihedral angles of 62.80 (6), 36.98 (6), 33.16 (6) and 46.24 (6)°, respectively, with the substituent rings in the 1-, 2-, 4- and 5-positions. No classical hydrogen bonds are observed in the crystal structure.

### Related literature

For the synthesis and pharmacological evaluation of substituted 1H-imidazoles, see: (Nagalakshmi, 2008). For contact allergy to imidazoles used as antimycotic agents, see: Dooms-Goossens *et al.* (1995). For related structures and applications of imidazole derivatives, see: Gayathri *et al.* (2010a,b,c).



### Experimental

#### Crystal data

 $\text{C}_{27}\text{H}_{19}\text{FN}_2$ 
 $M_r = 390.44$ 

Triclinic,  $P\bar{1}$   
 $a = 10.1794$  (5) Å  
 $b = 10.5239$  (6) Å  
 $c = 10.6175$  (6) Å  
 $\alpha = 80.750$  (5)°  
 $\beta = 85.776$  (4)°  
 $\gamma = 67.348$  (5)°

$V = 1035.95$  (11) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 295$  K  
 $0.51 \times 0.44 \times 0.15$  mm

#### Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer  
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)  
 $T_{\min} = 0.973$ ,  $T_{\max} = 1.000$

15513 measured reflections  
8350 independent reflections  
3489 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$   
 $wR(F^2) = 0.128$   
 $S = 0.86$   
8350 reflections

271 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.19$  e Å<sup>-3</sup>

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

JJ is thankful to the Department of Science and Technology [No. SR/S1/IC-07/2007] and the University Grants Commission (F. No. 36–21/2008 (SR)) for providing funds for this research. RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase an X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2707).

### References

- Dooms-Goossens, A., Matura, M., Drieghe, J. & Degreeef, H. (1995). *Contact Dermatitis*, **33**, 73–77.  
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
Gayathri, P., Jayabharathi, J., Saravanan, K., Thiruvalluvar, A. & Butcher, R. J. (2010a). *Acta Cryst.* **E66**, o1791.  
Gayathri, P., Jayabharathi, J., Srinivasan, N., Thiruvalluvar, A. & Butcher, R. J. (2010b). *Acta Cryst.* **E66**, o1703.  
Gayathri, P., Thiruvalluvar, A., Saravanan, K., Jayabharathi, J. & Butcher, R. J. (2010c). *Acta Cryst.* **E66**, o2219.  
Nagalakshmi, G. (2008). *Eur. J. Chem.* **5**, 447–452.  
Oxford Diffraction (2010). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, England.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

## supporting information

*Acta Cryst.* (2010). E66, o2519 [doi:10.1107/S1600536810035464]

**2-(4-Fluorophenyl)-1,4,5-triphenyl-1*H*-imidazole**

**P. Gayathri, A. Thiruvalluvar, N. Srinivasan, J. Jayabharathi and R. J. Butcher**

**S1. Comment**

Nagalakshmi (2008) has reported synthesis and pharmacological evaluation of 2-(4-Halo substituted phenyl)-4,5-diphenyl-1*H*-imidazoles, and Dooms-Goossens *et al.* (1995) have reported contact allergy to imidazoles used as antimycotic agents. As part of our research (Gayathri *et al.*, (2010*a,b,c*)), we have synthesized the title compound (I) and report its crystal structure here.

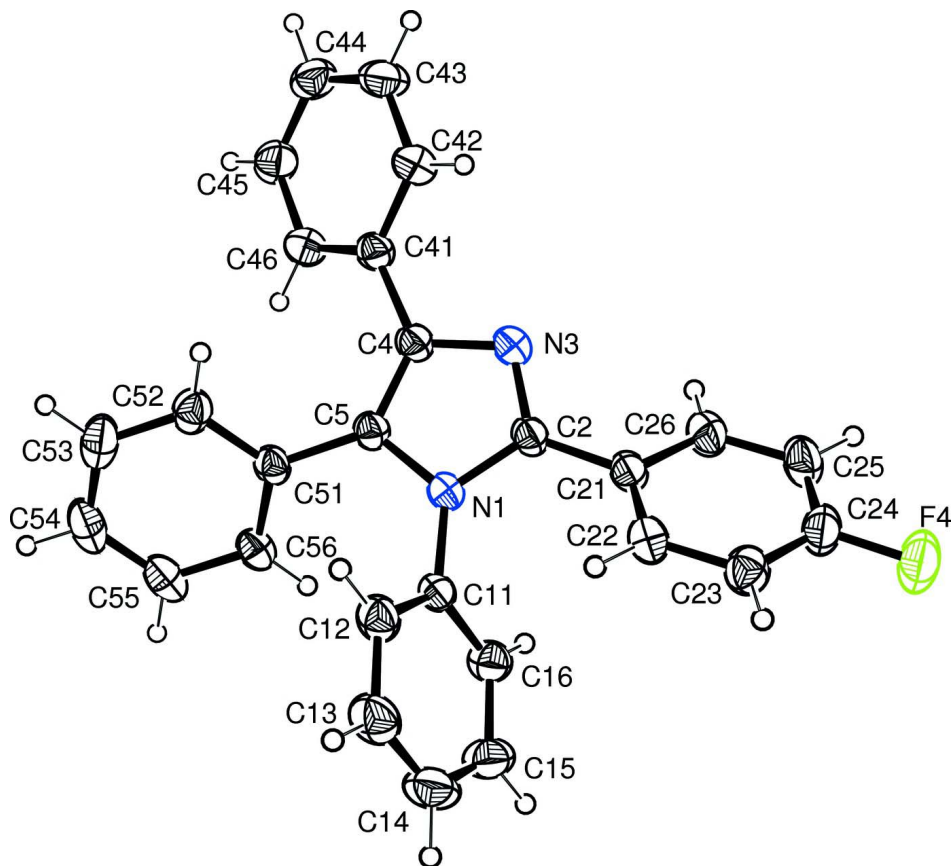
In (I), Fig. 1, the imidazole ring is essentially planar [maximum deviation = 0.004 (1) Å for N1]. The imidazole ring makes dihedral angles of 62.80 (6), 36.98 (6), 33.16 (6) and 46.24 (6) ° with the phenyl (C11—C16) attached to N1, fluorophenyl (C21—C26) attached to C2, and two phenyl rings (C41—C46) & (C51—C56) attached to C4 and C5, respectively. The phenyl ring at N1 makes dihedral angles of 54.26 (6), 85.21 (7) and 65.02 (6) ° with the fluorophenyl at C2, and phenyl rings attached to C4 and C5, respectively. The fluorophenyl ring makes dihedral angles of 63.01 (6) and 78.99 (6) ° with the phenyl rings at C4 and C5, respectively. Finally, the dihedral angle between the phenyl rings at C4 and C5 is 51.10 (6) °. In the crystal structure no classical hydrogen bonds are observed.

**S2. Experimental**

To benzil (3.15 g, 15 mmol) in ethanol (10 ml), aniline (1.5 g, 15 mmol), ammonium acetate (7 g, 15 mmol) and *p*-fluorobenzaldehyde (1.7 g, 15 mmol) were added over about 1 h while maintaining the temperature at 333 K. The reaction mixture was refluxed for 7 days and extracted with dichloromethane. The solid that separated was purified by column chromatography using hexane: ethyl acetate as the eluent. Yield: 3.51 g (60%).

**S3. Refinement**

H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.93 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$ .

**Figure 1**

The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius.

## 2-(4-Fluorophenyl)-1,4,5-triphenyl-1H-imidazole

### Crystal data

$C_{27}H_{19}FN_2$   
 $M_r = 390.44$   
 Triclinic,  $P\bar{1}$   
 Hall symbol: -P 1  
 $a = 10.1794$  (5) Å  
 $b = 10.5239$  (6) Å  
 $c = 10.6175$  (6) Å  
 $\alpha = 80.750$  (5)°  
 $\beta = 85.776$  (4)°  
 $\gamma = 67.348$  (5)°  
 $V = 1035.95$  (11) Å<sup>3</sup>

$Z = 2$   
 $F(000) = 408$   
 $D_x = 1.252$  Mg m<sup>-3</sup>  
 Melting point: 509 K  
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å  
 Cell parameters from 3942 reflections  
 $\theta = 5.1$ – $34.9$ °  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 295$  K  
 Plate, colourless  
 $0.51 \times 0.44 \times 0.15$  mm

### Data collection

Oxford Diffraction Xcalibur Ruby Gemini  
 diffractometer  
 Radiation source: Enhance (Mo) X-ray Source  
 Graphite monochromator  
 Detector resolution: 10.5081 pixels mm<sup>-1</sup>  
 $\omega$  scans

Absorption correction: multi-scan  
 (*CrysAlis PRO*; Oxford Diffraction, 2010)  
 $T_{\min} = 0.973$ ,  $T_{\max} = 1.000$   
 15513 measured reflections  
 8350 independent reflections  
 3489 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$   
 $\theta_{\text{max}} = 35.0^\circ$ ,  $\theta_{\text{min}} = 5.1^\circ$   
 $h = -15 \rightarrow 12$

$k = -16 \rightarrow 14$   
 $l = -17 \rightarrow 16$

### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.049$   
 $wR(F^2) = 0.128$   
 $S = 0.86$   
 8350 reflections  
 271 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0586P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.22 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.19 \text{ e } \text{\AA}^{-3}$

### Special details

**Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
F4	0.80372 (8)	0.08837 (10)	-0.40649 (7)	0.0903 (3)
N1	0.26200 (8)	0.23531 (9)	-0.01235 (8)	0.0437 (3)
N3	0.42488 (8)	0.27540 (10)	0.08546 (8)	0.0497 (3)
C2	0.39877 (10)	0.23282 (11)	-0.01679 (10)	0.0459 (3)
C4	0.30225 (10)	0.30605 (11)	0.15929 (9)	0.0455 (3)
C5	0.19960 (10)	0.28135 (11)	0.10135 (9)	0.0429 (3)
C11	0.20194 (9)	0.18684 (11)	-0.10385 (9)	0.0439 (3)
C12	0.16843 (11)	0.07116 (13)	-0.06763 (11)	0.0556 (4)
C13	0.11969 (13)	0.01955 (16)	-0.15797 (15)	0.0743 (5)
C14	0.10664 (14)	0.08323 (18)	-0.28296 (15)	0.0794 (6)
C15	0.14007 (13)	0.19852 (16)	-0.31824 (12)	0.0715 (5)
C16	0.18572 (11)	0.25319 (13)	-0.22810 (11)	0.0560 (4)
C21	0.50330 (10)	0.19099 (12)	-0.12073 (10)	0.0477 (3)
C22	0.51945 (10)	0.08114 (12)	-0.18562 (11)	0.0528 (4)
C23	0.62124 (11)	0.04652 (13)	-0.28141 (11)	0.0590 (4)
C24	0.70603 (12)	0.12091 (15)	-0.30998 (11)	0.0625 (4)
C25	0.69616 (13)	0.22763 (16)	-0.24730 (12)	0.0694 (5)
C26	0.59330 (12)	0.26275 (14)	-0.15231 (11)	0.0607 (4)
C41	0.30110 (11)	0.35537 (12)	0.28205 (10)	0.0468 (3)
C42	0.42822 (12)	0.30638 (14)	0.34878 (11)	0.0602 (4)
C43	0.43495 (14)	0.35356 (16)	0.46073 (12)	0.0713 (5)
C44	0.31579 (15)	0.44905 (16)	0.50961 (12)	0.0688 (5)
C45	0.19033 (14)	0.49726 (14)	0.44586 (12)	0.0654 (5)

C46	0.18239 (12)	0.45176 (12)	0.33263 (11)	0.0554 (4)
C51	0.05103 (10)	0.30008 (11)	0.13802 (10)	0.0438 (3)
C52	0.01739 (12)	0.25395 (13)	0.26117 (11)	0.0549 (4)
C53	-0.12281 (14)	0.27662 (14)	0.29629 (13)	0.0693 (5)
C54	-0.23054 (13)	0.34450 (15)	0.20932 (15)	0.0724 (5)
C55	-0.19831 (11)	0.38917 (14)	0.08727 (13)	0.0638 (4)
C56	-0.05946 (10)	0.36777 (12)	0.05109 (11)	0.0510 (4)
H12	0.17852	0.02828	0.01676	0.0667*
H13	0.09574	-0.05792	-0.13455	0.0892*
H14	0.07489	0.04771	-0.34393	0.0952*
H15	0.13200	0.24004	-0.40303	0.0857*
H16	0.20515	0.33333	-0.25085	0.0672*
H22	0.46150	0.03061	-0.16453	0.0633*
H23	0.63160	-0.02634	-0.32557	0.0708*
H25	0.75675	0.27545	-0.26776	0.0832*
H26	0.58432	0.33573	-0.10885	0.0728*
H42	0.50945	0.24100	0.31717	0.0722*
H43	0.52075	0.32058	0.50362	0.0856*
H44	0.32052	0.48059	0.58545	0.0825*
H45	0.10930	0.56144	0.47900	0.0785*
H46	0.09631	0.48633	0.29000	0.0664*
H52	0.08926	0.20754	0.32054	0.0659*
H53	-0.14438	0.24575	0.37930	0.0831*
H54	-0.32448	0.35981	0.23351	0.0868*
H55	-0.27068	0.43437	0.02817	0.0766*
H56	-0.03911	0.39881	-0.03226	0.0612*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
F4	0.0761 (5)	0.1160 (7)	0.0732 (5)	-0.0356 (5)	0.0285 (4)	-0.0132 (5)
N1	0.0411 (4)	0.0500 (5)	0.0453 (5)	-0.0228 (4)	0.0001 (3)	-0.0076 (4)
N3	0.0443 (4)	0.0584 (6)	0.0520 (5)	-0.0254 (4)	-0.0013 (4)	-0.0083 (4)
C2	0.0411 (5)	0.0509 (7)	0.0499 (6)	-0.0229 (5)	0.0000 (4)	-0.0051 (5)
C4	0.0445 (5)	0.0491 (6)	0.0468 (6)	-0.0223 (5)	-0.0025 (4)	-0.0051 (5)
C5	0.0426 (5)	0.0447 (6)	0.0442 (5)	-0.0206 (4)	0.0001 (4)	-0.0046 (5)
C11	0.0387 (5)	0.0495 (6)	0.0472 (6)	-0.0196 (5)	0.0009 (4)	-0.0107 (5)
C12	0.0570 (6)	0.0552 (7)	0.0621 (7)	-0.0296 (6)	0.0038 (5)	-0.0103 (6)
C13	0.0762 (8)	0.0745 (9)	0.0928 (11)	-0.0446 (7)	0.0064 (7)	-0.0319 (8)
C14	0.0734 (8)	0.0955 (12)	0.0841 (10)	-0.0365 (8)	-0.0108 (7)	-0.0387 (9)
C15	0.0701 (8)	0.0869 (10)	0.0561 (8)	-0.0245 (8)	-0.0131 (6)	-0.0144 (7)
C16	0.0571 (6)	0.0572 (7)	0.0551 (7)	-0.0235 (6)	-0.0057 (5)	-0.0050 (5)
C21	0.0404 (5)	0.0545 (7)	0.0494 (6)	-0.0210 (5)	-0.0011 (4)	-0.0027 (5)
C22	0.0437 (5)	0.0523 (7)	0.0614 (7)	-0.0188 (5)	0.0039 (5)	-0.0062 (5)
C23	0.0524 (6)	0.0580 (8)	0.0604 (7)	-0.0144 (6)	0.0025 (5)	-0.0091 (6)
C24	0.0487 (6)	0.0770 (9)	0.0532 (7)	-0.0191 (6)	0.0092 (5)	-0.0017 (6)
C25	0.0587 (7)	0.0863 (10)	0.0723 (8)	-0.0427 (7)	0.0096 (6)	-0.0028 (7)
C26	0.0563 (6)	0.0712 (8)	0.0653 (7)	-0.0360 (6)	0.0062 (5)	-0.0127 (6)

C41	0.0512 (6)	0.0504 (6)	0.0466 (6)	-0.0287 (5)	-0.0033 (4)	-0.0032 (5)
C42	0.0540 (6)	0.0720 (9)	0.0595 (7)	-0.0282 (6)	-0.0073 (5)	-0.0093 (6)
C43	0.0750 (8)	0.0885 (10)	0.0608 (8)	-0.0413 (8)	-0.0212 (6)	-0.0043 (7)
C44	0.0920 (9)	0.0822 (10)	0.0509 (7)	-0.0515 (8)	-0.0007 (7)	-0.0146 (7)
C45	0.0749 (8)	0.0694 (9)	0.0625 (7)	-0.0356 (7)	0.0050 (6)	-0.0209 (6)
C46	0.0563 (6)	0.0572 (7)	0.0580 (7)	-0.0255 (6)	-0.0053 (5)	-0.0112 (6)
C51	0.0442 (5)	0.0435 (6)	0.0509 (6)	-0.0231 (5)	0.0041 (4)	-0.0125 (5)
C52	0.0611 (6)	0.0548 (7)	0.0552 (7)	-0.0291 (6)	0.0088 (5)	-0.0117 (5)
C53	0.0808 (9)	0.0690 (9)	0.0711 (8)	-0.0434 (7)	0.0320 (7)	-0.0235 (7)
C54	0.0520 (7)	0.0751 (9)	0.1043 (11)	-0.0360 (7)	0.0224 (7)	-0.0331 (8)
C55	0.0454 (6)	0.0611 (8)	0.0917 (9)	-0.0240 (6)	-0.0002 (6)	-0.0207 (7)
C56	0.0470 (6)	0.0503 (7)	0.0620 (7)	-0.0247 (5)	-0.0009 (5)	-0.0095 (5)

*Geometric parameters (Å, °)*

F4—C24	1.3626 (15)	C45—C46	1.3822 (18)
N1—C2	1.3798 (14)	C51—C52	1.3859 (16)
N1—C5	1.3905 (13)	C51—C56	1.3960 (16)
N1—C11	1.4370 (13)	C52—C53	1.386 (2)
N3—C2	1.3194 (14)	C53—C54	1.378 (2)
N3—C4	1.3798 (14)	C54—C55	1.367 (2)
C2—C21	1.4718 (15)	C55—C56	1.3779 (17)
C4—C5	1.3759 (15)	C12—H12	0.9300
C4—C41	1.4761 (15)	C13—H13	0.9300
C5—C51	1.4785 (16)	C14—H14	0.9300
C11—C12	1.3771 (16)	C15—H15	0.9300
C11—C16	1.3793 (15)	C16—H16	0.9300
C12—C13	1.381 (2)	C22—H22	0.9300
C13—C14	1.378 (2)	C23—H23	0.9300
C14—C15	1.372 (2)	C25—H25	0.9300
C15—C16	1.3825 (19)	C26—H26	0.9300
C21—C22	1.3897 (16)	C42—H42	0.9300
C21—C26	1.3887 (18)	C43—H43	0.9300
C22—C23	1.3834 (17)	C44—H44	0.9300
C23—C24	1.3621 (19)	C45—H45	0.9300
C24—C25	1.363 (2)	C46—H46	0.9300
C25—C26	1.3843 (19)	C52—H52	0.9300
C41—C42	1.3950 (18)	C53—H53	0.9300
C41—C46	1.3831 (17)	C54—H54	0.9300
C42—C43	1.3755 (18)	C55—H55	0.9300
C43—C44	1.374 (2)	C56—H56	0.9300
C44—C45	1.365 (2)		
F4...H14 <sup>i</sup>	2.7400	C42...H54 <sup>i</sup>	2.9300
F4...H53 <sup>ii</sup>	2.7400	C44...H16 <sup>vi</sup>	2.9800
N1...H22	2.9400	C45...H25 <sup>vii</sup>	3.0000
N1...H56	2.8800	C46...H52	3.0900
N3...H26	2.6800	C51...H12	3.1000

N3...H42	2.5900	C51...H46	2.9100
N3...H55 <sup>iii</sup>	2.9400	C52...H46	2.9200
C2...C22 <sup>iv</sup>	3.4772 (16)	C53...H44 <sup>viii</sup>	2.9800
C4...C23 <sup>iv</sup>	3.5258 (17)	C53...H13 <sup>ix</sup>	3.0100
C5...C56 <sup>iii</sup>	3.5569 (16)	C54...H13 <sup>ix</sup>	3.0100
C5...C23 <sup>iv</sup>	3.5260 (16)	C54...H44 <sup>viii</sup>	2.9400
C11...C56	3.1419 (16)	C56...H56 <sup>iii</sup>	2.9700
C11...C22	3.0928 (15)	H12...C5	3.0300
C12...C51	3.3300 (16)	H12...C51	3.1000
C12...C56	3.4599 (17)	H13...C53 <sup>ix</sup>	3.0100
C16...C21	3.2942 (17)	H13...C54 <sup>ix</sup>	3.0100
C16...C22	3.2012 (17)	H14...F4 <sup>x</sup>	2.7400
C21...C16	3.2942 (17)	H16...C2	3.0700
C22...C11	3.0928 (15)	H16...C44 <sup>v</sup>	2.9800
C22...C2 <sup>iv</sup>	3.4772 (16)	H22...N1	2.9400
C22...C16	3.2012 (17)	H22...C11	2.6200
C23...C4 <sup>iv</sup>	3.5258 (17)	H22...C12	2.9700
C23...C5 <sup>iv</sup>	3.5260 (16)	H22...C16	2.9200
C41...C52	3.4747 (18)	H22...C2 <sup>iv</sup>	3.0100
C46...C51	3.4230 (16)	H23...C4 <sup>iv</sup>	3.0400
C46...C52	3.3345 (18)	H25...C45 <sup>vii</sup>	3.0000
C51...C46	3.4230 (16)	H26...N3	2.6800
C51...C12	3.3300 (16)	H42...N3	2.5900
C52...C46	3.3345 (18)	H42...H54 <sup>i</sup>	2.5000
C52...C41	3.4747 (18)	H43...C24 <sup>vi</sup>	2.8400
C56...C11	3.1419 (16)	H44...C53 <sup>viii</sup>	2.9800
C56...C56 <sup>iii</sup>	3.4379 (16)	H44...C54 <sup>viii</sup>	2.9400
C56...C5 <sup>iii</sup>	3.5569 (16)	H46...C5	3.0200
C56...C12	3.4599 (17)	H46...C51	2.9100
C2...H22 <sup>iv</sup>	3.0100	H46...C52	2.9200
C2...H16	3.0700	H52...C4	3.0500
C4...H55 <sup>iii</sup>	3.0300	H52...C41	3.0800
C4...H23 <sup>iv</sup>	3.0400	H52...C46	3.0900
C4...H52	3.0500	H53...F4 <sup>xi</sup>	2.7400
C5...H46	3.0200	H54...C42 <sup>x</sup>	2.9300
C5...H12	3.0300	H54...H42 <sup>x</sup>	2.5000
C11...H56	2.7600	H55...N3 <sup>iii</sup>	2.9400
C11...H22	2.6200	H55...C4 <sup>iii</sup>	3.0300
C12...H22	2.9700	H56...N1	2.8800
C16...H22	2.9200	H56...C11	2.7600
C16...H56	3.0900	H56...C16	3.0900
C24...H43 <sup>v</sup>	2.8400	H56...C56 <sup>iii</sup>	2.9700
C41...H52	3.0800		
C2—N1—C5	107.30 (9)	C52—C53—C54	120.60 (13)
C2—N1—C11	125.41 (9)	C53—C54—C55	119.52 (13)
C5—N1—C11	127.07 (9)	C54—C55—C56	120.53 (12)
C2—N3—C4	106.26 (9)	C51—C56—C55	120.81 (11)

N1—C2—N3	110.82 (9)	C11—C12—H12	120.00
N1—C2—C21	125.85 (9)	C13—C12—H12	120.00
N3—C2—C21	123.32 (10)	C12—C13—H13	120.00
N3—C4—C5	110.51 (9)	C14—C13—H13	120.00
N3—C4—C41	118.29 (10)	C13—C14—H14	120.00
C5—C4—C41	131.20 (10)	C15—C14—H14	120.00
N1—C5—C4	105.11 (9)	C14—C15—H15	120.00
N1—C5—C51	122.73 (9)	C16—C15—H15	120.00
C4—C5—C51	132.12 (9)	C11—C16—H16	121.00
N1—C11—C12	119.53 (9)	C15—C16—H16	121.00
N1—C11—C16	119.13 (10)	C21—C22—H22	120.00
C12—C11—C16	121.26 (10)	C23—C22—H22	120.00
C11—C12—C13	119.27 (11)	C22—C23—H23	121.00
C12—C13—C14	119.78 (14)	C24—C23—H23	121.00
C13—C14—C15	120.59 (14)	C24—C25—H25	121.00
C14—C15—C16	120.18 (12)	C26—C25—H25	121.00
C11—C16—C15	118.87 (12)	C21—C26—H26	119.00
C2—C21—C22	123.50 (10)	C25—C26—H26	119.00
C2—C21—C26	117.88 (10)	C41—C42—H42	120.00
C22—C21—C26	118.59 (10)	C43—C42—H42	120.00
C21—C22—C23	120.38 (11)	C42—C43—H43	120.00
C22—C23—C24	118.91 (12)	C44—C43—H43	120.00
F4—C24—C23	118.56 (12)	C43—C44—H44	120.00
F4—C24—C25	118.58 (12)	C45—C44—H44	120.00
C23—C24—C25	122.85 (12)	C44—C45—H45	120.00
C24—C25—C26	118.04 (13)	C46—C45—H45	120.00
C21—C26—C25	121.21 (12)	C41—C46—H46	120.00
C4—C41—C42	118.31 (11)	C45—C46—H46	120.00
C4—C41—C46	123.79 (11)	C51—C52—H52	120.00
C42—C41—C46	117.86 (11)	C53—C52—H52	120.00
C41—C42—C43	120.84 (13)	C52—C53—H53	120.00
C42—C43—C44	120.44 (14)	C54—C53—H53	120.00
C43—C44—C45	119.41 (13)	C53—C54—H54	120.00
C44—C45—C46	120.75 (13)	C55—C54—H54	120.00
C41—C46—C45	120.70 (12)	C54—C55—H55	120.00
C5—C51—C52	120.62 (10)	C56—C55—H55	120.00
C5—C51—C56	121.15 (9)	C51—C56—H56	120.00
C52—C51—C56	118.21 (11)	C55—C56—H56	120.00
C51—C52—C53	120.33 (12)		
C5—N1—C2—N3	-0.64 (12)	C16—C11—C12—C13	0.98 (18)
C5—N1—C2—C21	-179.79 (10)	N1—C11—C16—C15	174.19 (11)
C11—N1—C2—N3	-175.57 (9)	C12—C11—C16—C15	-2.50 (18)
C11—N1—C2—C21	5.28 (17)	C11—C12—C13—C14	0.7 (2)
C2—N1—C5—C4	0.72 (11)	C12—C13—C14—C15	-0.8 (2)
C2—N1—C5—C51	178.72 (10)	C13—C14—C15—C16	-0.8 (2)
C11—N1—C5—C4	175.54 (10)	C14—C15—C16—C11	2.4 (2)
C11—N1—C5—C51	-6.46 (16)	C2—C21—C22—C23	-179.20 (11)



C2—N1—C11—C12	112.68 (12)	C26—C21—C22—C23	-1.36 (17)
C2—N1—C11—C16	-64.07 (15)	C2—C21—C26—C25	178.74 (12)
C5—N1—C11—C12	-61.25 (15)	C22—C21—C26—C25	0.78 (18)
C5—N1—C11—C16	122.00 (12)	C21—C22—C23—C24	0.66 (18)
C4—N3—C2—N1	0.28 (12)	C22—C23—C24—F4	-178.45 (11)
C4—N3—C2—C21	179.46 (10)	C22—C23—C24—C25	0.7 (2)
C2—N3—C4—C5	0.20 (12)	F4—C24—C25—C26	177.87 (12)
C2—N3—C4—C41	179.33 (10)	C23—C24—C25—C26	-1.3 (2)
N1—C2—C21—C22	-38.85 (17)	C24—C25—C26—C21	0.5 (2)
N1—C2—C21—C26	143.30 (11)	C4—C41—C42—C43	177.03 (12)
N3—C2—C21—C22	142.10 (12)	C46—C41—C42—C43	-0.48 (19)
N3—C2—C21—C26	-35.75 (16)	C4—C41—C46—C45	-177.52 (12)
N3—C4—C5—N1	-0.57 (12)	C42—C41—C46—C45	-0.15 (18)
N3—C4—C5—C51	-178.31 (11)	C41—C42—C43—C44	0.7 (2)
C41—C4—C5—N1	-179.56 (11)	C42—C43—C44—C45	-0.2 (2)
C41—C4—C5—C51	2.7 (2)	C43—C44—C45—C46	-0.4 (2)
N3—C4—C41—C42	-31.76 (15)	C44—C45—C46—C41	0.6 (2)
N3—C4—C41—C46	145.60 (12)	C5—C51—C52—C53	177.49 (11)
C5—C4—C41—C42	147.16 (13)	C56—C51—C52—C53	-0.79 (18)
C5—C4—C41—C46	-35.48 (19)	C5—C51—C56—C55	-177.69 (11)
N1—C5—C51—C52	135.85 (11)	C52—C51—C56—C55	0.59 (17)
N1—C5—C51—C56	-45.92 (16)	C51—C52—C53—C54	0.4 (2)
C4—C5—C51—C52	-46.76 (18)	C52—C53—C54—C55	0.3 (2)
C4—C5—C51—C56	131.48 (13)	C53—C54—C55—C56	-0.5 (2)
N1—C11—C12—C13	-175.70 (11)	C54—C55—C56—C51	0.1 (2)

Symmetry codes: (i)  $x+1, y, z$ ; (ii)  $x+1, y, z-1$ ; (iii)  $-x, -y+1, -z$ ; (iv)  $-x+1, -y, -z$ ; (v)  $x, y, z-1$ ; (vi)  $x, y, z+1$ ; (vii)  $-x+1, -y+1, -z$ ; (viii)  $-x, -y+1, -z+1$ ; (ix)  $-x, -y, -z$ ; (x)  $x-1, y, z$ ; (xi)  $x-1, y, z+1$ .