

Crystal Structure Report for GT_DINESH_BI1_25022020

A Block-like specimen of $C_{18}H_{12}F_3N$, approximate dimensions 0.250 mm x 0.310 mm x 0.350 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured ($\lambda = 0.71073 \text{ \AA}$).

The total exposure time was 1.50 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 25820 reflections to a maximum θ angle of 29.92° (0.71 \AA resolution), of which 4165 were independent (average redundancy 6.199, completeness = 97.8%, $R_{\text{int}} = 9.32\%$, $R_{\text{sig}} = 7.00\%$) and 1735 (41.66%) were greater than $2\sigma(F^2)$. The final cell constants of $a = 12.049(6) \text{ \AA}$, $b = 7.905(5) \text{ \AA}$, $c = 30.896(15) \text{ \AA}$, volume = $2943.(3) \text{ \AA}^3$, are based upon the refinement of the XYZ-centroids of 3715 reflections above $20 \sigma(I)$ with $5.274^\circ < 2\theta < 58.04^\circ$. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.871. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6497 and 0.7460.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group Pbc_a , with $Z = 8$ for the formula unit, $C_{18}H_{12}F_3N$. The final anisotropic full-matrix least-squares refinement on F^2 with 199 variables converged at $R1 = 9.47\%$, for the observed data and $wR2 = 40.10\%$ for all data. The goodness-of-fit was 1.183. The largest peak in the final difference electron density synthesis was $0.795 \text{ e}^-/\text{\AA}^3$ and the largest hole was $-0.569 \text{ e}^-/\text{\AA}^3$ with an RMS deviation of $0.097 \text{ e}^-/\text{\AA}^3$. On the basis of the final model, the calculated density was 1.351 g/cm^3 and $F(000)$, 1248 e^- .

Table 1. Sample and crystal data for GT_DINESH_BI1_25022020.

Identification code	GT_DINESH_BI1_25022020	
Chemical formula	C ₁₈ H ₁₂ F ₃ N	
Formula weight	299.29 g/mol	
Wavelength	0.71073 Å	
Crystal size	0.250 x 0.310 x 0.350 mm	
Crystal system	orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 12.049(6) Å	α = 90°
	b = 7.905(5) Å	β = 90°
	c = 30.896(15) Å	γ = 90°
Volume	2943.(3) Å ³	
Z	8	
Density (calculated)	1.351 g/cm ³	
Absorption coefficient	0.106 mm ⁻¹	
F(000)	1248	

Table 2. Data collection and structure refinement for GT_DINESH_BI1_25022020.

Theta range for data collection	2.14 to 29.92°	
Index ranges	-15 ≤ h ≤ 15, -11 ≤ k ≤ 11, -43 ≤ l ≤ 43	
Reflections collected	25820	
Independent reflections	4165 [R(int) = 0.0932]	
Coverage of independent reflections	97.8%	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.7460 and 0.6497	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)	
Refinement method	Full-matrix least-squares on F ²	
Refinement program	olex2.refine 1.3 (Bourhis et al., 2015)	
Function minimized	Σ w(F _o ² - F _c ²) ²	
Data / restraints / parameters	4165 / 0 / 199	
Goodness-of-fit on F ²	1.183	
Δ/σ _{max}	0.784	
Final R indices	1735 data; I > 2σ(I)	R1 = 0.0947, wR2 = 0.2791
	all data	R1 = 0.1958, wR2 = 0.4010
Weighting scheme	w = 1/[σ ² (F _o ²) + (0.2P) ²] where P = (F _o ² + 2F _c ²)/3	
Largest diff. peak and hole	0.795 and -0.569 eÅ ⁻³	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å²) for GT_DINESH_BI1_25022020.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
F1	0.1158(4)	0.9303(5)	0.50615(12)	0.1677(18)
F2	0.1071(5)	0.6880(6)	0.53332(11)	0.202(3)
F3	0.2551(4)	0.7979(7)	0.52157(11)	0.1679(19)
N1	0.3450(2)	0.6334(4)	0.36654(9)	0.0621(8)
C1	0.6235(4)	0.7660(5)	0.23503(13)	0.0799(13)
C2	0.5183(4)	0.7952(5)	0.25277(13)	0.0717(11)
C3	0.4907(3)	0.7353(4)	0.29302(11)	0.0615(10)
C4	0.5431(3)	0.5722(4)	0.36057(11)	0.0546(9)
C5	0.4358(3)	0.5805(4)	0.38260(11)	0.0578(9)
C6	0.2491(3)	0.6356(4)	0.39328(12)	0.0595(9)
C7	0.2503(3)	0.7009(5)	0.43516(11)	0.0620(10)
C8	0.1539(3)	0.7027(5)	0.46010(13)	0.0659(10)
C9	0.0564(4)	0.6382(6)	0.44328(15)	0.0834(13)
C10	0.0541(4)	0.5768(6)	0.40138(17)	0.0886(14)
C11	0.1502(3)	0.5767(5)	0.37584(14)	0.0729(11)
C12	0.6262(3)	0.4868(5)	0.38274(12)	0.0662(10)
C13	0.7326(3)	0.4628(5)	0.36548(14)	0.0735(11)
C14	0.7572(3)	0.5263(5)	0.32507(13)	0.0694(11)
C15	0.6763(3)	0.6144(4)	0.30049(11)	0.0584(9)
C16	0.5679(3)	0.6404(4)	0.31823(10)	0.0522(8)
C17	0.7006(4)	0.6775(5)	0.25815(13)	0.0732(11)
C18	0.1548(4)	0.7752(6)	0.50472(15)	0.0819(13)

Table 4. Bond lengths (Å) for GT_DINESH_BI1_25022020.

F1-C18	1.314(5)	F2-C18	1.259(5)
F3-C18	1.328(6)	N1-C5	1.272(4)
N1-C6	1.420(4)	C1-H1	0.93
C1-C2	1.400(6)	C1-C17	1.365(6)
C2-H2	0.93	C2-C3	1.371(5)
C3-H3	0.93	C3-C16	1.427(5)
C4-C5	1.463(5)	C4-C12	1.388(5)
C4-C16	1.446(5)	C5-H5	0.93
C6-C7	1.393(5)	C6-C11	1.389(5)
C7-H7	0.93	C7-C8	1.394(5)
C8-C9	1.382(6)	C8-C18	1.493(6)
C9-H9	0.93	C9-C10	1.383(7)
C10-H10	0.93	C10-C11	1.401(6)

C11-H11	0.93	C12-H12	0.93
C12-C13	1.401(5)	C13-H13	0.93
C13-C14	1.378(5)	C14-H14	0.93
C14-C15	1.418(5)	C15-C16	1.431(5)
C15-C17	1.431(5)	C17-H17	0.93

**Table 5. Bond angles (°) for
GT_DINESH_BI1_25022020.**

C6-N1-C5	118.5(3)	C2-C1-H1	120.1(2)
C17-C1-H1	120.1(2)	C17-C1-C2	119.8(4)
H2-C2-C1	119.4(2)	C3-C2-C1	121.1(4)
C3-C2-H2	119.4(2)	H3-C3-C2	119.4(2)
C16-C3-C2	121.3(3)	C16-C3-H3	119.4(2)
C12-C4-C5	115.5(3)	C16-C4-C5	126.0(3)
C16-C4-C12	118.6(3)	C4-C5-N1	126.4(3)
H5-C5-N1	116.8(2)	H5-C5-C4	116.80(19)
C7-C6-N1	122.5(3)	C11-C6-N1	117.9(3)
C11-C6-C7	119.5(3)	H7-C7-C6	119.7(2)
C8-C7-C6	120.6(4)	C8-C7-H7	119.7(2)
C9-C8-C7	119.8(4)	C18-C8-C7	120.6(4)
C18-C8-C9	119.7(4)	H9-C9-C8	120.0(2)
C10-C9-C8	119.9(4)	C10-C9-H9	120.0(3)
H10-C10-C9	119.7(3)	C11-C10-C9	120.7(4)
C11-C10-H10	119.7(3)	C10-C11-C6	119.4(4)
H11-C11-C6	120.3(2)	H11-C11-C10	120.3(3)
H12-C12-C4	118.7(2)	C13-C12-C4	122.5(3)
C13-C12-H12	118.7(2)	H13-C13-C12	120.3(2)
C14-C13-C12	119.5(4)	C14-C13-H13	120.3(2)
H14-C14-C13	119.5(2)	C15-C14-C13	121.1(3)
C15-C14-H14	119.5(2)	C16-C15-C14	119.5(3)
C17-C15-C14	121.4(3)	C17-C15-C16	119.1(3)
C4-C16-C3	123.7(3)	C15-C16-C3	117.5(3)
C15-C16-C4	118.8(3)	C15-C17-C1	121.2(4)
H17-C17-C1	119.4(2)	H17-C17-C15	119.4(2)
F2-C18-F1	108.9(5)	F3-C18-F1	100.7(5)
F3-C18-F2	102.4(5)	C8-C18-F1	112.8(4)
C8-C18-F2	115.8(4)	C8-C18-F3	114.8(4)

**Table 6. Torsion angles (°) for
GT_DINESH_BI1_25022020.**

F1-C18-C8-C7	99.4(4)	F1-C18-C8-C9	-80.1(5)
F2-C18-C8-C7	-134.3(5)	F2-C18-C8-C9	46.3(6)
F3-C18-C8-C7	-15.2(5)	F3-C18-C8-C9	165.3(4)
N1-C5-C4-C12	-170.9(4)	N1-C5-C4-C16	7.5(4)
N1-C6-C7-C8	179.1(3)	N1-C6-C11-C10	179.9(4)
C1-C2-C3-C16	-0.3(5)	C1-C17-C15-C14	-178.3(4)
C1-C17-C15-C16	1.9(4)	C2-C3-C16-C4	-179.1(3)
C2-C3-C16-C15	1.8(4)	C3-C16-C4-C5	3.9(4)

C3-C16-C4-C12	-177.8(3)	C3-C16-C15-C14	177.6(3)
C3-C16-C15-C17	-2.6(4)	C4-C12-C13-C14	0.3(4)
C4-C16-C15-C14	-1.5(3)	C4-C16-C15-C17	178.3(3)
C6-C7-C8-C9	0.4(4)	C6-C7-C8-C18	-179.0(4)
C6-C11-C10-C9	1.4(5)	C7-C8-C9-C10	-1.9(4)
C8-C9-C10-C11	1.0(5)	C12-C13-C14-C15	-0.6(5)
C13-C14-C15-C16	1.1(4)	C13-C14-C15-C17	-178.7(4)

Table 7. Anisotropic atomic displacement parameters (\AA^2) for GT_DINESH_BI1_25022020.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	0.255(5)	0.134(3)	0.115(3)	-0.030(2)	0.000(3)	0.075(3)
F2	0.318(7)	0.201(5)	0.088(2)	-0.013(2)	0.068(3)	-0.135(5)
F3	0.135(3)	0.261(6)	0.107(3)	-0.076(3)	0.001(2)	0.009(3)
N1	0.0531(19)	0.0702(18)	0.0631(17)	-0.0002(14)	0.0075(14)	-0.0020(14)
C1	0.096(3)	0.084(3)	0.059(2)	0.0079(19)	0.012(2)	-0.012(2)
C2	0.078(3)	0.071(2)	0.066(2)	0.0112(18)	-0.004(2)	-0.0006(19)
C3	0.061(2)	0.065(2)	0.0582(19)	0.0032(16)	-0.0009(17)	-0.0010(16)
C4	0.054(2)	0.0541(17)	0.0552(18)	-0.0056(14)	0.0000(15)	-0.0037(15)
C5	0.061(2)	0.0572(18)	0.0557(19)	0.0030(15)	0.0028(16)	-0.0020(16)
C6	0.055(2)	0.0584(19)	0.065(2)	0.0081(16)	0.0090(17)	0.0010(15)
C7	0.059(2)	0.061(2)	0.067(2)	0.0077(17)	0.0057(17)	0.0008(16)
C8	0.063(2)	0.058(2)	0.077(2)	0.0110(17)	0.0164(19)	0.0035(17)
C9	0.071(3)	0.084(3)	0.096(3)	0.008(2)	0.026(2)	0.002(2)
C10	0.059(3)	0.097(3)	0.110(4)	0.013(3)	0.000(2)	-0.012(2)
C11	0.066(3)	0.076(2)	0.076(3)	0.005(2)	-0.001(2)	-0.0047(19)
C12	0.067(3)	0.069(2)	0.062(2)	0.0028(17)	-0.0057(17)	0.0043(18)
C13	0.064(3)	0.073(2)	0.084(3)	0.002(2)	-0.012(2)	0.0105(19)
C14	0.055(2)	0.067(2)	0.086(2)	-0.012(2)	0.0039(18)	0.0078(17)
C15	0.056(2)	0.0576(19)	0.0611(19)	-0.0091(15)	0.0005(16)	-0.0051(16)
C16	0.052(2)	0.0491(16)	0.0549(18)	-0.0041(14)	0.0008(14)	-0.0029(14)
C17	0.067(3)	0.078(2)	0.075(2)	-0.007(2)	0.019(2)	-0.008(2)
C18	0.081(3)	0.088(3)	0.076(3)	0.001(2)	0.023(2)	0.005(2)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (\AA^2) for GT_DINESH_BI1_25022020.

	x/a	y/b	z/c	U(eq)
H1	0.6407(4)	0.8067(5)	0.2076(13)	0.0959(15)
H2	0.4661(4)	0.8562(5)	0.2370(13)	0.0860(13)
H3	0.4204(3)	0.7571(4)	0.3041(11)	0.0738(11)
H5	0.4337(3)	0.5435(4)	0.4112(11)	0.0694(11)

	x/a	y/b	z/c	U(eq)
H7	0.3160(3)	0.7436(5)	0.4466(11)	0.0745(12)
H9	-0.0075(4)	0.6361(6)	0.4601(15)	0.1001(15)
H10	-0.0120(4)	0.5352(6)	0.3900(17)	0.1064(16)
H11	0.1477(3)	0.5376(5)	0.3475(14)	0.0875(13)
H12	0.6107(3)	0.4439(5)	0.4101(12)	0.0794(12)
H13	0.7862(3)	0.4045(5)	0.3812(14)	0.0881(13)
H14	0.8280(3)	0.5112(5)	0.3137(13)	0.0833(13)
H17	0.7703(4)	0.6579(5)	0.2462(13)	0.0878(13)

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Datablock: GT_DINESH_BI1_25022020_0m_a

Bond precision: C-C = 0.0055 A Wavelength=0.71073
 Cell: a=12.049(6) b=7.905(5) c=30.896(15)
 alpha=90 beta=90 gamma=90

Temperature: 303 K

	Calculated	Reported
Volume	2943(3)	2943(3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C18 H12 F3 N	C18 H12 F3 N
Sum formula	C18 H12 F3 N	C18 H12 F3 N
Mr	299.29	299.29
Dx,g cm-3	1.351	1.351
Z	8	8
Mu (mm-1)	0.106	0.106
F000	1232.0	1232.0
F000'	1232.75	
h,k,lmax	16,11,43	15,11,43
Nref	4258	4170
Tmin,Tmax	0.964,0.975	0.650,0.746
Tmin'	0.964	

Correction method= # Reported T Limits: Tmin=0.650 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 0.979

Theta(max)= 29.916

R(reflections)= 0.0915(1738)

wR2(reflections)= 0.3755(4170)

S = 0.976

Npar= 199

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

[PLAT084_ALERT_3_B](#) High wR2 Value (i.e. > 0.25)

0.38 Report

Alert level C

[ABSTY02_ALERT_1_C](#) An _expt1_absorpt_correction_type has been given without a literature citation. This should be contained in the _expt1_absorpt_process_details field.

Absorption correction given as Multi-Scan

[CRYSC01_ALERT_1_C](#) No recognised colour has been given for crystal colour.

[DIFMN02_ALERT_2_C](#) The minimum difference density is < -0.1*ZMAX*0.75

_refine_diff_density_min given = -0.788
 Test value = -0.675

[DIFMN03_ALERT_1_C](#) The minimum difference density is < -0.1*ZMAX*0.75
 The relevant atom site should be identified.
[PLAT026_ALERT_3_C](#) Ratio Observed / Unique Reflections (too) Low .. 42% Check
[PLAT098_ALERT_2_C](#) Large Reported Min. (Negative) Residual Density -0.79 eA-3
[PLAT340_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.00547 Ang.

Alert level G

[PLAT072_ALERT_2_G](#) SHELXL First Parameter in WGHT Unusually Large 0.20 Report
[PLAT242_ALERT_2_G](#) Low MainMol Ueq as Compared to Neighbors of C18 Check
[PLAT883_ALERT_1_G](#) No Info/Value for _atom_sites_solution_primary . Please Do !

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 1 **ALERT level B** = A potentially serious problem, consider carefully
 - 7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 3 **ALERT level G** = General information/check it is not something unexpected
-
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 3 ALERT type 3 Indicator that the structure quality may be low
 - 0 ALERT type 4 Improvement, methodology, query or suggestion
 - 0 ALERT type 5 Informative message, check

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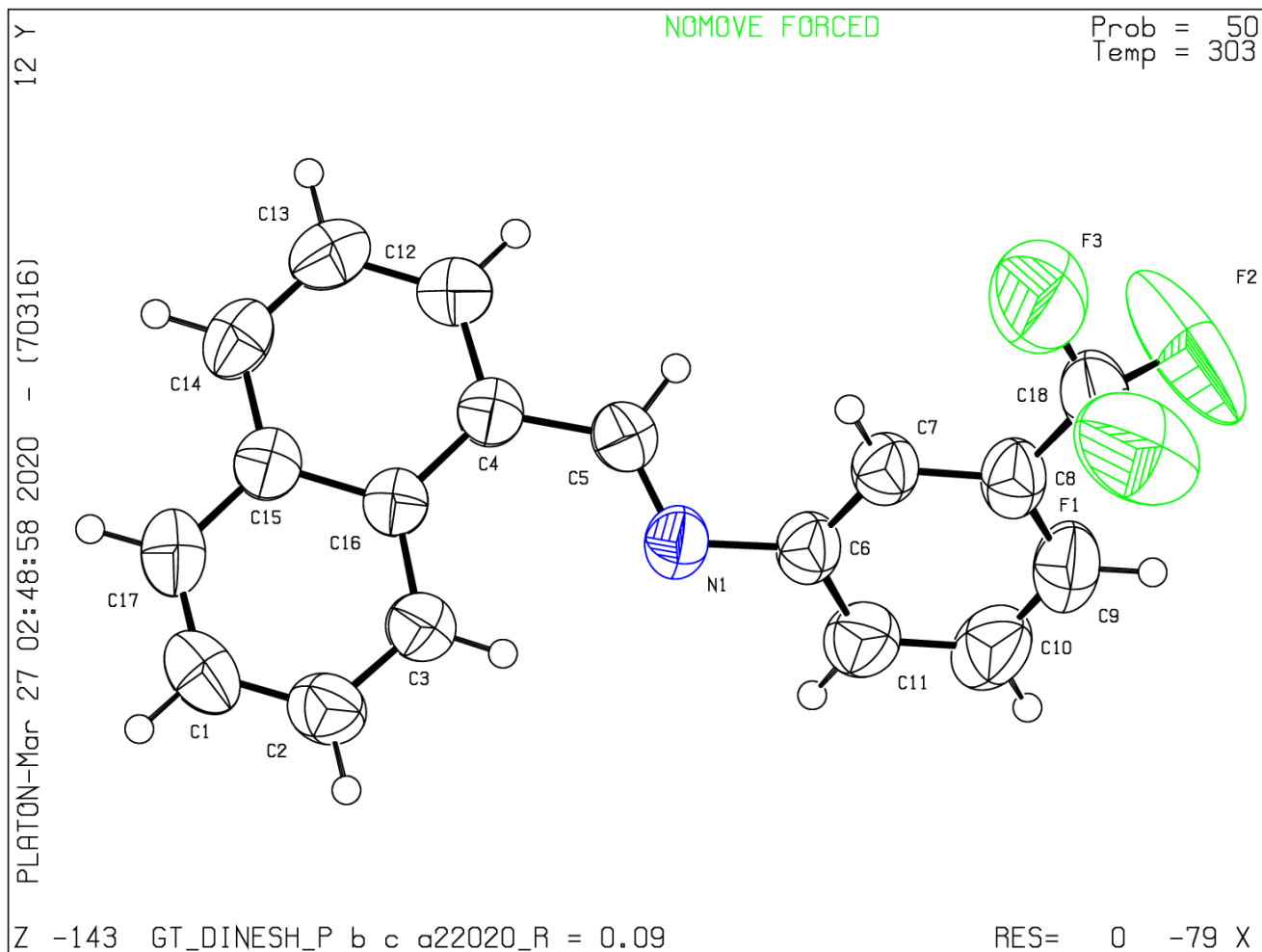
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Datablock GT_DINESH_BI1_25022020_0m_a - ellipsoid plot



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