



## Supporting Information

for

### Configuration–packing synergy enabling integrated crystalline-state RTP and amorphous-state TADF

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### Checkcif file for compound 1



## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 19090503

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. [CIF dictionary](#) [Interpreting this report](#)

### Datablock: 19090503

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Bond precision: C-C = 0.0023 Å Wavelength=1.54184

Cell: a=8.6894 (2) b=35.8672 (5) c=8.1002 (1)  
alpha=90 beta=107.351 (2) gamma=90

Temperature: 220 K

	Calculated	Reported
Volume	2409.67 (8)	2409.67 (8)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moietiy formula	C33 H22 N2 O2	C33 H22 N2 O2
Sum formula	C33 H22 N2 O2	C33 H22 N2 O2
Mr	478.53	478.52
D <sub>x</sub> , g cm <sup>-3</sup>	1.319	1.319
Z	4	4
μ (mm <sup>-1</sup> )	0.653	0.653
F <sub>000</sub>	1000.0	1000.0
F <sub>000'</sub>	1002.87	
h, k, lmax	10, 44, 10	10, 43, 9
N <sub>ref</sub>	4831	4617
T <sub>min</sub> , T <sub>max</sub>	0.889, 0.974	0.297, 1.000
T <sub>min'</sub>	0.861	

Correction method= # Reported T Limits: T<sub>min</sub>=0.297 T<sub>max</sub>=1.000  
AbsCorr = MULTI-SCAN

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 C

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.116 Check  
 PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STH/L= 0.600 48 Report  
   1 0 0, 2 0 0, 3 0 0, 0 20 0, 0 22 0, 0 24 0,  
   6 34 0, 2 1 1, 0 22 1, -1 23 1, 0 23 1, -1 24 1,  
   0 24 1, 0 0 2, 1 0 2, 2 0 2, 0 1 2, 0 22 2,  
 -10 1 5, -10 2 5, 4 0 6, 5 0 6, 5 1 6, 5 2 6,  
   5 3 6, -9 11 6, -9 12 6, -9 13 6, -9 14 6, -8 21 6,  
   ( 18 More Missing: see the .ckf listing file)

#### • Alert level G

PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 59 Note  
 0001 0002 N003 N004 C005 C006 C007 C008  
 C009 H009 C00A C00B C00C C00D H00D C00E  
 C00F H00F C00G H00G C00H C00I H00I C00J  
 H00J C00K H00K C00L H00L C00M H00M C00N  
 C00O C00P H00P C00Q C00R C00S H00S C00T  
 H00T C00U H00U C00V H00V C00W H00W C00X  
 H00X C00Y H00Y C00Z H00A H00B H00C C010  
 H010 C011 H011

PLAT910\_ALERT\_3\_G Missing FCF Reflection(s) Below Theta(Min) [Deg] = 4.93 Note  
 0 2 0,

PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L = 0.600 152 Note

PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 1.7 Low

PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 2.785 Note

Predicted wR2: Based on SigI\*\*2 5.13 or SHELX Weight 14.32

PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 16 Info

PLAT992 ALERT 5 G Repd & Actual reflns number qt Values Differ by 2 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

**ALERT level C** = Check. Ensure it is not caused by an omission or oversight.

**ALERT level C** = Check. Ensure it is not caused by an omission or oversight.  
**ALERT level G** = General information/check it is not something unexpected.

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

1 ALERT type 1 Off construction, by-pass effect, inconsistent or missing data  
1 ALERT type 2 Indicator that the structure model may be wrong or deficient

1 ALERT type 2 Indicator that the structure model may be wrong  
4 ALERT type 3 Indicator that the structure quality may be low

2 ALERT type 4 Improvement, methodology, query or suggestion

2 ALERT type 4 Improvement, methodology, 0  
3 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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**PLATON version of 26/09/2025; check.def file version of 20/09/2025**

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## **duplicate check**

**No duplication found**

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Datablock 19090503 - ellipsoid plot

