



## Supporting Information

for

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

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*Beilstein J. Org. Chem.* **2026**, 22, 224–236. doi:10.3762/bjoc.22.16

## 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) alpha=90	b=35.8672 (5) beta=107.351 (2)
Temperature:	220 K	c=8.1002 (1) gamma=90
	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
Moiety formula	C33 H22 N2 O2	C33 H22 N2 O2
Sum formula	C33 H22 N2 O2	C33 H22 N2 O2
Mr	478.53	478.52
Dx, g cm <sup>-3</sup>	1.319	1.319
Z	4	4
Mu (mm <sup>-1</sup> )	0.653	0.653
F000	1000.0	1000.0
F000'	1002.87	
h, k, lmax	10, 44, 10	10, 43, 9
Nref	4831	4617
Tmin, Tmax	0.889, 0.974	0.297, 1.000
Tmin'	0.861	

Correction method= # Reported T Limits: Tmin=0.297 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.956

Theta(max)= 73.323

R(reflections)= 0.0489( 4070)

wR2(reflections)=  
0.1427( 4617)

S = 0.997

Npar= 335

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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.

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### ● 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)

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### ● Alert level G

PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 59 Note

O001	O002	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\_gt Values Differ by 2 Check

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **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 2 Indicator that the structure model may be wrong or deficient  
4 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check
- 
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**PLATON version of 26/09/2025; check.def file version of 20/09/2025**

## No duplication found

PLATON-Oct 1 9:25:03 2025 - (VERSION=260925)

40 Y

NOMOVE FORCED

Prob = 50%  
Temp = 220K

ORTEP diagram of a complex organic molecule, likely a carboxylate salt or a complex organic acid derivative. The structure features a central core with a nitrogen atom (N004) and a disordered region (N003). The molecule is shown in a stick representation with thermal ellipsoids at the 50% probability level. The structure includes several carboxylate groups (COO) and a central core with a nitrogen atom (N004) and a disordered region (N003). The molecule is shown in a stick representation with thermal ellipsoids at the 50% probability level. The structure includes several carboxylate groups (COO) and a central core with a nitrogen atom (N004) and a disordered region (N003).

Z -158 19090503 P 1 21/c 1 R = 0.05 RES= 0-121 X