



## checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 20230525d\_auto

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Bond precision:	C-C = 0.0060 Å	Wavelength=1.54184	
Cell:	a=12.5350 (4) alpha=90	b=5.2858 (2) beta=96.963 (3)	c=14.2151 (5) gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	934.91 (6)	934.91 (6)	
Space group	P 21	P 1 21 1	
Hall group	P 2yb	P 2yb	
Moiety formula	C27 H18 N3	C27 H18 N3	
Sum formula	C27 H18 N3	C27 H18 N3	
Mr	384.44	384.44	
Dx, g cm <sup>-3</sup>	1.366	1.366	
Z	2	2	
Mu (mm <sup>-1</sup> )	0.633	0.633	
F000	402.0	402.0	
F000'	403.09		
h, k, lmax	15, 6, 17	15, 6, 17	
Nref	3917 [ 2178]	2923	
Tmin, Tmax	0.796, 0.909	0.795, 1.000	
Tmin'	0.729		

Correction method= # Reported T Limits: Tmin=0.795 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.34/0.75           Theta(max)= 76.384

R(reflections)= 0.0546( 2319)

wR2(reflections)=  
0.1495( 2923)

S = 1.100

Npar= 271

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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**

ABSTY02\_ALERT\_1\_C An `_exptl_absorpt_correction_type` has been given without a literature citation. This should be contained in the `_exptl_absorpt_process_details` field.

Absorption correction given as multi-scan

STRVA01\_ALERT\_4\_C           Flack test results are meaningless.

From the CIF: `_refine_ls_abs_structure_Flack`    0.100

From the CIF: `_refine_ls_abs_structure_Flack_su`   0.900

PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds .....    0.00603 Ang.

PLAT790\_ALERT\_4\_C Centre of Gravity not Within Unit-Cell: Resd. #           1 Note  
                  C27 H18 N3

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● **Alert level G**

PLAT012\_ALERT\_1\_G No           `_shelx_res_checksum` Found in CIF .....    Please Check

PLAT032\_ALERT\_4\_G Std. Uncertainty on Flack Parameter Value High .    0.900 Report

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File        35 Note

          -9 1 13, -9 -1 13, -7 1 13, -7 -1 13, -6 -2 11, -11 0 13,

          -10 0 13, -10 -1 13, -10 1 13, -12 0 12, -12 -1 12, -11 -2 11,

          -12 1 12, -13 -1 11, -10 -2 11, -10 1 12, -10 -1 12, -13 1 11,

          -11 -1 12, -13 0 11, -12 -2 10, -12 1 11, -12 -1 11, -14 0 10,

          -11 0 12, 1 1 2, 10 -1 6, -11 -2 10, 10 1 6, 6 -1 6,

          -13 -2 7, -11 -2 9, -13 -1 10, -11 0 7, 7 -1 7,

PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity .....        3.0 Low

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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

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

4 **ALERT level G** = General information/check it is not something unexpected

2 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

2 ALERT type 3 Indicator that the structure quality may be low

3 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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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.

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

## duplicate check

No duplication found

Datablock 20230525d\_auto - ellipsoid plot

