



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) yd_ms_bcb_1930_0m_a

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: yd_ms_bcb_1930_0m_a

Bond precision:	C-C = 0.0019 Å	Wavelength=0.71073	
Cell:	a=8.2701 (19) alpha=90	b=12.237 (3) beta=97.872 (8)	c=13.439 (3) gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	1347.2 (5)	1347.3 (5)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C17 H17 N O2	4 (C17 H17 N O2)	
Sum formula	C17 H17 N O2	C68 H68 N4 O8	
Mr	267.32	1069.26	
Dx, g cm ⁻³	1.318	1.318	
Z	4	1	
Mu (mm ⁻¹)	0.086	0.086	
F000	568.0	568.0	
F000'	568.25		
h, k, lmax	11, 16, 18	11, 16, 18	
Nref	3520	3459	
Tmin, Tmax	0.992, 0.998	0.678, 0.746	
Tmin'	0.988		

Correction method= # Reported T Limits: Tmin=0.678 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.983

Theta(max)= 28.848

R(reflections)= 0.0481(2784)

wR2(reflections)=
0.1290(3459)

S = 1.051

Npar= 190

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**

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: C17 H17 N O2
Rep.: C68 H68 N4 O8

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C17 H17 N O2
Rep.: 4(C17 H17 N O2)

PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 23 Report

0	2	0,	1	3	0,	0	4	0,	1	4	0,	-3	0	1,	-3	1	1,
1	3	1,	-1	4	1,	-2	5	1,	-2	1	2,	1	1	2,	-1	2	2,
-2	7	2,	1	0	3,	0	1	3,	0	0	4,	1	1	4,	-3	3	4,
0	1	5,	2	2	5,	-1	2	6,	1	0	7,	0	0	8,			

● **Alert level G**

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 4 Check

PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O002 . 105.9 Degree

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 34 Note

O001	O002	N003	C004	C005	H005	C006	C007
H00A	H00B	C008	H00C	H00D	C00A	H00E	C00B
H00F	C00C	H00G	C00D	H00H	C00E	C00F	H00I
C00G	H00J	C00H	C00I	C00J	H00K	C00K	H00L
H00M	H00N						

PLAT793_ALERT_4_G Model has Chirality at C00C (Centro SpGr) S Verify

PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 2.74 Note

0 1 1,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 37 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 3 Note

1 0 3, 0 0 4, 1 0 7,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 20 Note

-3	0	1,	-3	1	1,	-3	3	4,	-2	1	2,	-2	5	1,	-2	7	2,
-1	2	2,	-1	2	6,	0	0	4,	0	1	1,	0	1	3,	0	1	5,
0	2	0,	0	4	0,	1	0	3,	1	1	2,	1	3	0,	1	3	1,
1	4	0,	2	2	5,												

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.369 Note

Predicted wR2: Based on SigI**2 3.83 or SHELX Weight 12.28

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 13 Info

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

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 3 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
- 4 ALERT type 4 Improvement, methodology, query or suggestion
- 1 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.

PLATON version of 04/06/2025; check.def file version of 30/05/2025

Datablock yd_ms_bcb_1930_0m_a - ellipsoid plot

