



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) jz_001

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: jz_001

Bond precision:	C-C = 0.0026 Å	Wavelength=1.54184
Cell:	a=5.4986 (1) alpha=90	b=9.7302 (1) beta=90
Temperature:	100 K	c=31.0562 (4) gamma=90
	Calculated	Reported
Volume	1661.58 (4)	1661.58 (4)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C17 H26 O4	C17 H26 O4
Sum formula	C17 H26 O4	C17 H26 O4
Mr	294.38	294.38
Dx, g cm ⁻³	1.177	1.177
Z	4	4
Mu (mm ⁻¹)	0.665	0.665
F000	640.0	640.0
F000'	641.95	
h, k, lmax	6, 12, 39	6, 12, 39
Nref	3477 [2052]	3362
Tmin, Tmax	0.961, 0.987	0.487, 1.000
Tmin'	0.858	

Correction method= # Reported T Limits: Tmin=0.487 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.64/0.97

Theta(max)= 76.314

R(reflections)= 0.0339(3141)

wR2(reflections)=
0.0911(3362)

S = 1.044

Npar= 195

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 G

PLAT791_ALERT_4_G Model has Chirality at C1	(Sohncke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C2	(Sohncke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C6	(Sohncke SpGr)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C8	(Sohncke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C10	(Sohncke SpGr)	R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600	36 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value		2.259 Note
Predicted wR2: Based on SigI**2	4.03 or SHELX Weight	8.73 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		2 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **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
0 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
1 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 23/04/2026; check.def file version of 30/03/2026

