



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) jz

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

Bond precision:	C-C = 0.0105 Å	Wavelength=1.54184
Cell:	a=6.4304 (2) alpha=90	b=11.4726 (5) beta=93.661 (3) c=27.031 (1) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	1990.10 (13)	1990.10 (13)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C20 H32 O5	C20 H32 O5
Sum formula	C20 H32 O5	C20 H32 O5
Mr	352.46	352.45
Dx, g cm ⁻³	1.176	1.176
Z	4	4
Mu (mm ⁻¹)	0.671	0.671
F000	768.0	768.0
F000'	770.35	
h, k, lmax	8, 14, 34	8, 14, 33
Nref	8388 [4412]	6994
Tmin, Tmax	0.982, 0.993	0.581, 1.000
Tmin'	0.948	

Correction method= # Reported T Limits: Tmin=0.581 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.59/0.83

Theta(max)= 76.672

R(reflections)= 0.0765(6258)

wR2(reflections)=
0.1798(6994)

S = 1.115

Npar= 480

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 B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01053 Ang.



Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.105 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 53 Report

4	9	0,	2	13	0,	5	0	1,	6	7	1,	-4	9	1,	4	9	1,
-3	10	1,	-2	13	1,	2	13	1,	6	6	2,	6	7	2,	4	9	2,
-4	10	2,	-2	13	2,	6	7	3,	4	9	3,	-4	10	3,	-3	10	3,
-2	13	3,	6	6	4,	6	7	4,	-3	10	4,	-3	11	4,	-2	11	4,
-2	13	4,	6	6	5,	-3	10	5,	-2	11	5,	-1	12	5,	-2	13	5,

(23 More Missing: see the .ckf listing file)



Alert level G

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 8 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 3 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0001 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0001 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0001 Report
PLAT301_ALERT_3_G Main Residue Disorder (Resd 1) 4% Note
PLAT791_ALERT_4_G Model has Chirality at C2 (Sohncke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C5 (Sohncke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C7 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C8 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C9 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C14 (Sohncke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C15 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C17 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C24 (Sohncke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C25 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C27 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C30 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C37 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C38 (Sohncke SpGr) R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints 43 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 3.28 Note
0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 157 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.15 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law [1 0 4] Est.d BASF 0.34 Check

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 6 Note
 -5 1 2, -3 1 3, 0 -1 7, 4 -8 3, 4 -7 0, 5 0 1,
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.7 Low
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.246 Note
 Predicted wR2: Based on SigI**2 5.54 or SHELX Weight 16.13

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 29 **ALERT level G** = General information/check it is not something unexpected

0 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
 10 ALERT type 3 Indicator that the structure quality may be low
 17 ALERT type 4 Improvement, methodology, query or suggestion
 2 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 17/09/2025; check.def file version of 17/09/2025

