



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 12.17_auto

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: 12.17_auto

Bond precision:	C-C = 0.0051 Å	Wavelength=1.54184	
Cell:	a=10.1331 (1)	b=10.1331 (1)	c=20.9219 (3)
	alpha=90	beta=90	gamma=120
Temperature:	100 K		
	Calculated	Reported	
Volume	1860.44 (5)	1860.44 (5)	
Space group	P 32 2 1	P 32 2 1	
Hall group	P 32 2 "	P 32 2 "	
Moiety formula	C22 H28 Br2 Co O2 P2	C22 H28 Br2 Co O2 P2	
Sum formula	C22 H28 Br2 Co O2 P2	C22 H28 Br2 Co O2 P2	
Mr	605.11	605.13	
Dx, g cm ⁻³	1.620	1.620	
Z	3	3	
Mu (mm ⁻¹)	10.540	10.540	
F000	909.0	909.0	
F000'	901.24		
h, k, lmax	12, 12, 26	12, 12, 26	
Nref	2611 [1526]	2522	
Tmin, Tmax	0.182, 0.349	0.563, 1.000	
Tmin'	0.081		

Correction method= # Reported T Limits: Tmin=0.563 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.65/0.97 Theta(max)= 76.327

R(reflections)= 0.0222(2458)

wR2(reflections)=
0.0522(2522)

S = 1.041

Npar= 136

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**

PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * Sigma from Zero .	0.198	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	29	Note
	Br01 Co02 P003 O004 C005 C006 C007 H007		
	C008 H008 C009 H00A H00B C00A H00C C00B		
	C00C H00D H00E H00F C00D C00E H00G H00H		
	H00I C00F H00J H00K H00L		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	32	Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.003	Note
	Predicted wR2: Based on SigI**2 2.61 or SHELX Weight	5.01	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info
PLAT994_ALERT_1_G	SHELXL .ins Contains no or MERG 0 Instruction ..		! Note

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

1 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
3 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 15/01/2026; check.def file version of 02/01/2026
