

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp\_2092

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: exp\_2092

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Bond precision:	C-C = 0.0047 A	Wavelength=1.54184
Cell:	a=9.8357(4)	b=11.2310(5)      c=16.6786(6)
	alpha=70.974(4)	beta=87.088(3)      gamma=67.371(4)
Temperature:	100 K	
	Calculated	Reported
Volume	1601.77(13)	1601.77(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H59 B Dy P	C32 H59 B Dy P
Sum formula	C32 H59 B Dy P	C32 H59 B Dy P
Mr	648.07	648.07
Dx,g cm-3	1.344	1.344
Z	2	2
Mu (mm-1)	13.053	13.053
F000	674.0	674.0
F000'	656.37	
h,k,lmax	11,13,19	11,13,19
Nref	5720	5711
Tmin,Tmax	0.261,0.676	0.289,1.000
Tmin'	0.167	

Correction method= # Reported T Limits: Tmin=0.289 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.998      Theta(max)= 67.077

R(reflections)= 0.0314( 5524)      wR2(reflections)= 0.0811( 5711)

S = 1.037      Npar= 334

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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.



### Alert level C

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PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.17	Report
PLAT410_ALERT_2_C	Short Intra H...H Contact H12 ..H15 .	1.94	Ang.
	x,y,z =	1_555	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.597	9 Report

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### Alert level G

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PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	1	Note
PLAT303_ALERT_2_G	Full Occupancy Atom H1A with # Connections	2.00	Check
PLAT303_ALERT_2_G	Full Occupancy Atom H1B with # Connections	2.00	Check
PLAT328_ALERT_4_G	Possible Missing H on sp3? Phosphorus .....	P1	Check
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	97%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	1.9	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

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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  
 3 **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  
 5 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 4 ALERT type 3 Indicator that the structure quality may be low  
 2 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. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock exp\_2092 - ellipsoid plot

