

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait ..

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) 1

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](#)
Please wait while processing [Interpreting this report](#)

[Structure factor report](#)

Datablock: 1

Bond precision:	C-C = 0.0078 A	Wavelength=0.71073
Cell:	a=15.482(3)	b=8.741(2)
	alpha=90	beta=98.382(10)
		gamma=90
Temperature: 193 K		
	Calculated	Reported
Volume	1373.6(5)	1373.7(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H20 N O P	C13 H20 N O P
Sum formula	C13 H20 N O P	C13 H20 N O P
Mr	237.27	237.27
Dx,g cm-3	1.147	1.147
Z	4	4
Mu (mm-1)	0.182	0.182
F000	512.0	512.0
F000'	512.58	
h,k,lmax	18,10,12	18,10,12
Nref	2491	2489
Tmin,Tmax	0.983,0.991	0.652,0.746
Tmin'	0.982	
Correction method= #	Reported T Limits: Tmin=0.652 Tmax=0.746	
AbsCorr = MULTI-SCAN		
Data completeness= 0.999	Theta(max)= 25.245	
R(reflections)= 0.0864(1754)	wR2(reflections)= 0.2003(2489)	
S = 1.113	Npar= 183	

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

- PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00775 Ang.
- PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 18.333 Check
- PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.057 Check
- PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report

Alert level G

- PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 9 Note
- PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 12 Report
- PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.41 Why ?

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0200 Report
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 38% Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 291 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 43% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.0 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.5 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
4 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. 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 10/05/2023; check.def file version of 10/05/2023

Datablock 1 - ellipsoid plot

