

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deh085_raj_sad

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: deh085_raj_sad

Bond precision:	C-C = 0.0062 A	Wavelength=0.71073
Cell:	a=15.1077(9)	b=20.1735(12) c=25.4559(16)
	alpha=90	beta=97.989(3) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	7683.0(8)	7683.0(8)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C38 H38 Fe N2 P, F6 P, C H2 Cl2	C38 H38 Fe N2 P, F6 P, C H2 Cl2
Sum formula	C39 H40 Cl2 F6 Fe N2 P2	C39 H40 Cl2 F6 Fe N2 P2
Mr	839.42	839.42
Dx,g cm-3	1.451	1.451
Z	8	8
Mu (mm-1)	0.676	0.676
F000	3456.0	3456.0
F000'	3464.28	
h,k,lmax	20,26,34	20,26,34
Nref	19210	19156
Tmin,Tmax	0.724,0.935	0.650,0.746
Tmin'	0.634	

Correction method= # Reported T Limits: Tmin=0.650 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 28.359

R(reflections)= 0.0675(13743) wR2(reflections)= 0.1897(19156)

S = 1.122 Npar= 952

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

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers 3 Check



Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C77 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00616 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 35 Ang3
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.986 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 6 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 3 Report
PLAT971_ALERT_2_C Check Calcd Residual Density 1.29A From Cl3 1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.44A From Cl3 -1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.87A From Cl3 -1.55 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density 0 Note



Alert level G

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size 0.66 mm
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 31.27 Why ?
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P3 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P4 Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 48 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
5 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.

