

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) GM5_22_0m

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: GM5_22_0m

Bond precision:	C-C = 0.0039 A	Wavelength=0.71073	
Cell:	a=13.0988 (5)	b=16.1147 (6)	c=20.7612 (7)
	alpha=90	beta=98.233 (1)	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	4337.2 (3)	4337.2 (3)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C50 H40 Cu N2 P2 S, B F4	?	
Sum formula	C50 H40 B Cu F4 N2 P2 S	C50 H40 B Cu F4 N2 P2 S	
Mr	913.20	913.19	
Dx, g cm ⁻³	1.398	1.398	
Z	4	4	
Mu (mm ⁻¹)	0.681	0.681	
F000	1880.0	1880.0	
F000'	1883.31		
h, k, lmax	15, 19, 24	15, 19, 24	
Nref	7649	7632	
Tmin, Tmax	0.728, 0.762	0.530, 0.600	
Tmin'	0.704		

Correction method= # Reported T Limits: Tmin=0.530 Tmax=0.600
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 24.999

R(reflections)= 0.0336 (6559)	wR2(reflections)= 0.0951 (7632)
S = 1.065	Npar= 587

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

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C2A	--C3A	.	6.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C5A	--C6A	.	5.9 s.u.
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	--P2C	.	9.0 s.u.
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	F1			0.107 Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).				9 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595			8 Report



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				9 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
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of				B1 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)				7% Note
PLAT722_ALERT_1_G	Angle Calc 122.00, Rep 120.70 Dev...				1.30 Degree
	C14D -C13D -H13D 1_555 1_555 1_555 #	162			Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	140			Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .				Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still				72% Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	3			Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	4			Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities				Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0			Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0			Info

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

- 2 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
6 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

