

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a

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: a

Bond precision:	C-C = 0.0143 A	Wavelength=1.34139	
Cell:	a=29.1614 (16) alpha=90	b=29.1614 (16) beta=90	c=29.1614 (16) gamma=90
Temperature:	173 K		
	Calculated	Reported	
Volume	24799 (4)	24798 (4)	
Space group	P -4 3 n	P -4 3 n	
Hall group	P -4n 2 3	P -4n 2 3	
Moiety formula	C312 H444 N4 O48 P24 Pt12 [+ solvent]	0.25 (C312 H444 N4 O48 P24 Pt12)	
Sum formula	C312 H444 N4 O48 P24 Pt12 [+ solvent]	C78 H111 N O12 P6 Pt3	
Mr	8102.96	2025.76	
Dx, g cm ⁻³	1.085	1.085	
Z	2	8	
Mu (mm ⁻¹)	4.949	4.950	
F000	8048.0	8048.0	
F000'	7943.13		
h, k, lmax	36, 36, 36	36, 36, 36	
Nref	8553 [4545]	8540	
Tmin, Tmax	0.580, 0.610	0.360, 0.751	
Tmin'	0.526		

Correction method= # Reported T Limits: Tmin=0.360 Tmax=0.751

AbsCorr = MULTI-SCAN

Data completeness= 1.88/1.00

Theta(max)= 57.243

R(reflections)= 0.0417(7453)

wR2(reflections)=
0.1192(8540)

S = 1.064

Npar= 317

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	3.2	Ratio
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared to Neighbors of		Pt1	Check
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds				0.01433	Ang.
PLAT412_ALERT_2_C	Short Intra XH3 ..	XHn	H23C	..H24B	.	1.88	Ang.
				x,y,z =		1_555	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between	Thmin & STh/L=	0.600			5	Report



Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu			not performed for this radiation type.			
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					10	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...					16	Report
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ					Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...					0.25	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records					1	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records					3	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records					5	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records					3	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records					1	Report
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)				3%	Note
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure					!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints					106	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600				2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...					6	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.					1	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
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
16 **ALERT level G** = General information/check it is not something unexpected
- 3 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
4 ALERT type 3 Indicator that the structure quality may be low
7 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.

