

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3-Ce

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: 3-Ce

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Bond precision:      C-C = 0.0161 Å

Wavelength=1.54178

Cell:                      a=11.405(5)                      b=13.149(9)                      c=20.917(15)  
                              alpha=85.025(15)                      beta=75.629(18)                      gamma=68.180(15)  
Temperature:      120 K

	Calculated	Reported
Volume	2821(3)	2821(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C56 H89 Ce O4 P4	C56 H89 Ce O4 P4
Sum formula	C56 H89 Ce O4 P4	C56 H89 Ce O4 P4
Mr	1090.27	1090.27
Dx, g cm <sup>-3</sup>	1.284	1.284
Z	2	2
Mu (mm <sup>-1</sup> )	7.623	7.624
F000	1150.0	1150.0
F000'	1151.19	
h,k,lmax	14,16,25	14,16,25
Nref	11165	10882
Tmin,Tmax	0.387,0.802	0.373,0.754
Tmin'	0.229	

Correction method= # Reported T Limits: Tmin=0.373 Tmax=0.754  
AbsCorr = MULTI-SCAN

Data completeness= 0.975

Theta(max)= 72.397

R(reflections)= 0.1027( 6779)

wR2(reflections)=  
0.2932( 10882)

S = 1.044

Npar= 790

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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.

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### Alert level C

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12  
Rint given 0.166

PLAT020\_ALERT\_3\_C The Value of Rint is Greater Than 0.12 ..... 0.166 Report

PLAT084\_ALERT\_3\_C High wR2 Value (i.e. > 0.25) ..... 0.29 Report

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Cel --O4A . 0.16 Ang.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of O3 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C31 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C29 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C39 Check

PLAT334\_ALERT\_2\_C Small <C-C> Benzene Dist. C29 -C34 . 1.37 Ang.

PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.01609 Ang.

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.917 Check

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 126 Report

12 1 0, 13 3 0, 13 4 0, 13 5 0, 13 8 0, 11 10 0,  
12 10 0, 11 11 0, 12 11 0, 11 12 0, -11-12 1, -12-11 1,  
-11-11 1, -12-10 1, -11-10 1, -12 -9 1, -13 -7 1, -13 -6 1,  
-13 -5 1, -13 -4 1, -12 -3 1, 12 2 1, 13 3 1, 11 4 1,  
13 4 1, 13 9 1, 11 10 1, 12 10 1, 11 11 1, 12 11 1,  
-11-12 2, -11-11 2, -12-10 2, -12 -9 2, -7 -6 2, -12 -4 2,  
-12 -3 2, 13 3 2, 12 11 2, 11 12 2, -11-12 3, -10-12 3,  
-11-11 3, -12-10 3, -12 -9 3, -12 -8 3, -12 -7 3, -12 -6 3,  
-12 -5 3, -12 -4 3, -12 -3 3, -11 -3 3, -12 -2 3, 13 3 3,  
12 11 3, 12 12 3, -11-11 4, -12 -9 4, -12 -8 4, -11 -8 4,  
-12 -7 4, -11 -7 4, -12 -6 4, -12 -5 4, -11 -5 4, -12 -4 4,  
-11 -4 4, -12 -3 4, -11 -3 4, -12 -2 4, 12 11 4, 12 12 4,  
-10-12 5, -11-11 5, -12 -8 5, -12 -7 5, -11 -7 5, -12 -6 5,  
-11 -6 5, -12 -5 5, -11 -5 5, -12 -4 5, -11 -4 5, -12 -3 5,  
-11 -3 5, -10 -3 5, -10-12 6, -11 -7 6, -12 -6 6, -11 -6 6,  
-12 -5 6, -11 -5 6, -10 -5 6, -12 -4 6, -11 -4 6, -10 -4 6,

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 1.05Ang From Cel 2.42 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.96Ang From Cel 1.60 eA-3

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 1.07Ang From Cel -2.23 eA-3

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.86Ang From Cel -1.62 eA-3

PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.75Ang From Ol . -0.54 eA-3



### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 39 Note

PLAT003\_ALERT\_2\_G Number of Uiso or U(i,j) Restrained non-H Atoms 39 Report

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 1 Report

H1

PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.16 Report

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 7.88 Why ?

PLAT175\_ALERT\_4\_G The CIF-Embedded .res File Contains SAME Records 1 Report

PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records 1 Report

PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 2 Report

PLAT187\_ALERT\_4\_G The CIF-Embedded .res File Contains RIGU Records 1 Report

PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1)	29%	Note
PLAT303_ALERT_2_G	Full Occupancy Atom H1	with # Connections	2.00	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H22C ..H54A .	2.07	Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H31 ..H38F .	1.77	Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H40A ..H36F .	1.83	Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H41C ..H38D .	1.76	Ang.
		x,y,z =	1_555	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		15.40	Deg.
	CE1 -P1 -H1	1_555 1_555 1_555 .....	# 21	Check
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters		5	Info
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....		!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		1246	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		157	Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....		2.742	Note
	Predicted wR2: Based on SigI**2 10.69 or SHELX Weight 28.08			
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  
 18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 24 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 21 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 10 ALERT type 3 Indicator that the structure quality may be low  
 8 ALERT type 4 Improvement, methodology, query or suggestion  
 3 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.

