

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: grot319

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Bond precision:	C-C = 0.0086 A	Wavelength=0.71073
Cell:	a=12.1218(10)	b=19.2680(15)      c=28.333(2)
	alpha=90	beta=90      gamma=90
Temperature:	200 K	
	Calculated	Reported
Volume	6617.5(9)	6617.6(9)
Space group	P b c n	Pbcn
Hall group	-P 2n 2ab	?
Moiety formula	2(C23 H32 Cl N3 Rh), 2(F6 P), 3(C4 H8 O)	?
Sum formula	C58 H88 Cl2 F12 N6 O3 P2 Rh2	C29 H44 Cl F6 N3 O1.50 P Rh
Mr	1484.00	742.00
Dx,g cm-3	1.490	1.490
Z	4	8
Mu (mm-1)	0.708	0.708
F000	3056.0	3056.0
F000'	3050.54	
h,k,lmax	14,22,33	14,22,33
Nref	5851	5840
Tmin,Tmax	0.820,0.880	0.826,0.883
Tmin'	0.820	

Correction method= # Reported T Limits: Tmin=0.826 Tmax=0.883  
AbsCorr = MULTI-SCAN

Data completeness= 0.998      Theta(max)= 25.030

R(reflections)= 0.0468( 4495)      wR2(reflections)= 0.1394( 5840)

S = 1.029      Npar= 393

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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.

### ● Alert level C

PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00856 Ang.
PLAT360_ALERT_2_C	Short C(sp <sup>3</sup> )-C(sp <sup>3</sup> ) Bond C28 - C29 .	1.43 Ang.

### ● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	13	Note
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		? Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	13.96	Why ?
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1 --F2 .	22.5	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1 --F3 .	11.0	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1 --F4 .	22.0	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1 --F5 .	11.0	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1 --F1A .	5.5	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1 --F2A .	19.5	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1 --F3A .	10.5	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1 --F4A .	19.0	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1 --F5A .	10.5	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1 --F6A .	6.0	s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P1	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	86%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1	103.0	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O2	105.0	Degree
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	168	Check
	F1A -P1 -F1 1.555 1.555 1.555	34.50	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	175	Check
	F3A -P1 -F3 1.555 1.555 1.555	9.80	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	180	Check
	F4 -P1 -F4A 1.555 1.555 1.555	33.70	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	193	Check
	F6 -P1 -F6A 1.555 1.555 1.555	40.70	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	201	Check
	F5 -P1 -F5A 1.555 1.555 1.555	9.10	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	210	Check
	F2A -P1 -F2 1.555 1.555 1.555	38.40	Deg.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3	Note
	C4 H8 O		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	36	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2017	Note

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

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

