

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) c\_\_maw281116

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: c\_\_maw281116

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Bond precision:    C-C = 0.0065 A

Wavelength=0.71073

Cell:                a=11.7074(3)                b=12.2413(4)                c=12.8682(3)  
                      alpha=89.647(2)        beta=75.623(2)        gamma=88.455(2)  
Temperature:        183 K

	Calculated	Reported
Volume	1785.79(9)	1785.79(9)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C29 H27 N3 O5 Re, F6 P, C4 H8 O	C33 H35 F6 N3 O6 P Re
Sum formula	C33 H35 F6 N3 O6 P Re	C33 H35 F6 N3 O6 P Re
Mr	900.82	900.81
Dx,g cm-3	1.675	1.675
Z	2	2
Mu (mm-1)	3.525	3.525
F000	892.0	892.0
F000'	890.68	
h,k,lmax	16,16,17	16,16,17
Nref	9995	9941
Tmin,Tmax	0.662,0.781	0.435,0.780
Tmin'	0.369	

Correction method= # Reported T Limits: Tmin=0.435 Tmax=0.780

AbsCorr = MULTI-SCAN

Data completeness= 0.995

Theta(max)= 29.570

R(reflections)= 0.0378( 8439)

wR2(reflections)= 0.0852( 9941)

S = 1.029

Npar= 454

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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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.32	Report
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	4.1	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C26	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C31	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	O32	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C30	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C34	Check
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C30 - C31 ..	1.43	Ang.
PLAT397_ALERT_2_C	Deviating C-O-C Angle from 120 Deg for O32	108.0	Degree
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	46	Report
PLAT971_ALERT_2_C	Check Calcd Residual Density 0.90A From Rel	1.82	eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density 0.93A From Rel	1.64	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Residual Density on Rel	1.39	eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on H31A	-0.57	eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Note

### ● Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please	Do !
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P1	Check
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	1	Do !
	C2 -RE1 -C1 -O1 -120.00 6.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	2	Do !
	C3 -RE1 -C1 -O1 -31.00 6.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	3	Do !
	N3 -RE1 -C1 -O1 152.00 6.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	4	Do !
	N2 -RE1 -C1 -O1 64.00 6.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	5	Do !
	N1 -RE1 -C1 -O1 48.00 6.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	6	Do !
	C1 -RE1 -C2 -O2 -78.00 8.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	7	Do !
	C3 -RE1 -C2 -O2 -162.00 8.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	8	Do !
	N3 -RE1 -C2 -O2 25.00 8.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	9	Do !
	N2 -RE1 -C2 -O2 71.00 8.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	10	Do !
	N1 -RE1 -C2 -O2 104.00 8.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	11	Do !
	C1 -RE1 -C3 -O3 -59.00 11.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	12	Do !
	C2 -RE1 -C3 -O3 30.00 11.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	13	Do !
	N3 -RE1 -C3 -O3 104.00 11.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	14	Do !
	N2 -RE1 -C3 -O3 -155.00 11.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	15	Do !
	N1 -RE1 -C3 -O3 131.00 11.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	16	Do !
	C1 -RE1 -N1 -C24 -138.40 0.70 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	21	Do !

C1 -RE1 -N1 -C4	-23.40	0.80	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							26 Do !
C1 -RE1 -N1 -C14	92.40	0.70	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							32 Do !
C2 -RE1 -N2 -C5	62.50	1.10	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							37 Do !
C2 -RE1 -N2 -C13	-124.10	1.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							43 Do !
C3 -RE1 -N3 -C15	31.40	1.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #							48 Do !
C3 -RE1 -N3 -C23	-144.00	0.80	1.555	1.555	1.555	1.555	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #							2 Note
F6 P							
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #							3 Note
C4 H8 O							
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL							2014 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)							4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600							12 Note

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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  
 15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 31 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 10 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  
 31 ALERT type 4 Improvement, methodology, query or suggestion  
 1 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.

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**PLATON version of 24/11/2016; check.def file version of 23/11/2016**

