

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) maw160817

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: maw160817

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Bond precision:	C-C = 0.0038 A	Wavelength=0.71073
Cell:	a=17.3858(4)      b=9.8329(2)      c=17.3855(4)	
	alpha=90      beta=110.109(2)      gamma=90	
Temperature:	160 K	
	Calculated	Reported
Volume	2790.92(11)	2790.92(11)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H23 N3 O4 Re, F6 P	C26 H23 N3 O4 Re, F6 P
Sum formula	C26 H23 F6 N3 O4 P Re	C26 H23 F6 N3 O4 P Re
Mr	772.65	772.64
Dx,g cm-3	1.839	1.839
Z	4	4
Mu (mm-1)	4.489	4.489
F000	1504.0	1504.0
F000'	1501.25	
h,k,lmax	24,14,24	24,14,24
Nref	8523	8524
Tmin,Tmax	0.592,0.727	0.617,0.741
Tmin'	0.580	

Correction method= # Reported T Limits: Tmin=0.617 Tmax=0.741  
AbsCorr = MULTI-SCAN

Data completeness= 1.000      Theta(max)= 30.508

R(reflections)= 0.0225( 7691)      wR2(reflections)= 0.0517( 8524)

S = 1.047      Npar= 371

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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**

PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	P1	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....		2.1	Note
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4	..F1	2.59	Ang.

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**Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....		1	Report
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent)	P1 --F1	5.2	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent)	P1 --F2	5.7	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent)	P1 --F3	5.4	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent)	P1 --F4	7.8	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent)	P1 --F5	5.9	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent)	P1 --F6	6.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Re1 --C1	6.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Re1 --C2	7.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Re1 --C3	7.4	s.u.
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		5	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  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
13 **ALERT level G** = General information/check it is not something unexpected

1 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  
1 ALERT type 3 Indicator that the structure quality may be low  
8 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.

