

# checkCIF/PLATON report

No syntax errors found.    CIF dictionary    Interpreting this report

## Datablock: phw1308

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Bond precision:    C-C = 0.0027 Å                      Wavelength=0.71070

Cell:                      a=19.0875(3)              b=12.10177(17)              c=24.0122(3)  
                                    alpha=90                      beta=90                      gamma=90

Temperature:              110 K

	Calculated	Reported
Volume	5546.64(14)	5546.65(15)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C30 H24 F9 N3	C30 H24 F9 N3
Sum formula	C30 H24 F9 N3	C30 H24 F9 N3
Mr	597.47	597.52
Dx,g cm-3	1.431	1.431
Z	8	8
Mu (mm-1)	0.127	0.127
F000	2447.8	2448.0
F000'	2449.57	
h,k,lmax	25,16,31	24,15,31
Nref	6709	5708
Tmin,Tmax	0.978,0.991	0.979,0.992
Tmin'	0.965	

Correction method= ANALYTICAL

Data completeness= 0.851                      Theta(max)= 28.030

R(reflections)= 0.0445( 4563)              wR2(reflections)= 0.1041( 5708)

S = 1.059                      Npar= 406

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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

PLAT068\_ALERT\_1\_C Reported F000 Differs from Calcd (or Missing)...              ? Check  
PLAT242\_ALERT\_2\_C Check Low              Ueq as Compared to Neighbors for              C30

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### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite              10

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF	? Do !
PLAT301_ALERT_3_G	Note: Main Residue Disorder	.....	7 %
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F4 .. F7B .	2.84 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F5 .. F7B .	2.62 Ang.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	.....	37

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
4 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  
0 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*, 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 01/06/2013; check.def file version of 24/05/2013**

