

Structure factors have been supplied for datablock(s) 1

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	C-C = 0.0039 Å	Wavelength=1.54178	
Cell:	a=16.4931(4)	b=14.5514(3)	c=15.3803(4)
	alpha=90	beta=115.620(2)	gamma=90
Temperature:	273 K		

```
Correction method= # Reported T Limits: Tmin=0.546 Tmax=0.753
AbsCorr = MULTI-SCAN
```

```
R(reflections)= 0.0535( 4760)      wR2(reflections)=
S = 1.074                        0.1649( 6098)
Npar= 397
```

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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

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: C20 H22 Cl N  
Rep.: 2(C20 H22 Cl N)

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C23 --C24 . 5.6 s.u.  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C27 --C31 . 6.3 s.u.  
PLAT410\_ALERT\_2\_C Short Intra H...H Contact H25 ..H32A . 1.94 Ang.  
x,y,z = 1\_555 Check

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 12.185 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 24 Report

-2 13 1, 0 14 1, 0 15 1, 5 16 1, -1 16 2, 0 3 2,  
0 14 2, -1 13 3, 1 14 3, 2 15 3, -4 13 4, 0 0 4,  
0 15 4, 1 14 4, -1 15 5, 0 15 5, 1 14 5, 2 15 5,  
0 14 6, 3 3 6, -1 15 7, 0 14 7, 3 1 7, -5 11 14,

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### Alert level G

PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 2 Check  
PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 273 Check  
PLAT200\_ALERT\_1\_G Reported \_diffn\_ambient\_temperature ..... (K) 273 Check  
PLAT793\_ALERT\_4\_G Model has Chirality at C10 (Centro SpGr) S Verify  
PLAT793\_ALERT\_4\_G Model has Chirality at C14 (Centro SpGr) S Verify  
PLAT793\_ALERT\_4\_G Model has Chirality at C27 (Centro SpGr) S Verify  
PLAT793\_ALERT\_4\_G Model has Chirality at C31 (Centro SpGr) S Verify  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 4 Note  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 4.472 Note  
Predicted wR2: Based on SigI\*\*2 3.69 or SHELX Weight 15.35  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 3 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  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
10 **ALERT level G** = General information/check it is not something unexpected

- 4 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  
5 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.

Datablock 1 - ellipsoid plot

