

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 201\_07\_13\_DS040\_white\_0m

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: 201\_07\_13\_DS040\_white\_0m

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Bond precision:    C-C = 0.0032 Å                      Wavelength=0.71073

Cell:                      a=8.2621(6)              b=18.7132(14)              c=17.9937(14)  
                            alpha=90              beta=93.326(1)              gamma=90  
Temperature:              125 K

	Calculated	Reported
Volume	2777.3(4)	2777.3(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C28 H39 Cl3 N2	?
Sum formula	C28 H39 Cl3 N2	C28 H39 Cl3 N2
Mr	509.96	509.96
Dx,g cm-3	1.220	1.220
Z	4	4
Mu (mm-1)	0.348	0.348
F000	1088.0	1088.0
F000'	1090.07	
h,k,lmax	10,23,22	10,23,22
Nref	5440	5405
Tmin,Tmax	0.847,0.852	0.597,0.746
Tmin'	0.847	

Correction method= # Reported T Limits: Tmin=0.597 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.994                      Theta(max)= 26.000

R(reflections)= 0.0466( 4508)              wR2(reflections)= 0.1287( 5405)

S = 1.045                      Npar= 306

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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 B

PLAT410\_ALERT\_2\_B Short Intra H...H Contact H2 .. H23 . 1.84 Ang.

**Author Response: Due to steric pressure from the CCl3 group on the adjacent isopropyl groups, the 2,6-diisopropylphenyl substituents on the opposite side are pushed towards the H2 atom resulting in these short intramolecular distances**



#### Alert level C

PLAT220\_ALERT\_2\_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio  
PLAT222\_ALERT\_3\_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 4.3 Ratio  
PLAT410\_ALERT\_2\_C Short Intra H...H Contact H2 .. H11 . 1.99 Ang.

**Author Response: Due to steric pressure from the CCl3 group on the adjacent isopropyl groups, the 2,6-diisopropylphenyl substituents on the opposite side are pushed towards the H2 atom resulting in these short intramolecular distances**

PLAT911\_ALERT\_3\_C Missing # FCF Refl Between THmin & STh/L= 0.600 29 Report



#### Alert level G

PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 6 Note  
PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 1 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 4 Info

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

0 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  
1 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

