

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compoundL3

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: compoundL3

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Bond precision:    C-C = 0.0064 Å                      Wavelength=0.71073

Cell:                      a=19.195(3)              b=8.5030(13)              c=30.611(5)  
                                alpha=90              beta=90              gamma=90  
Temperature:              100 K

	Calculated	Reported
Volume	4996.2(14)	4996.2(13)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C33 H26 N2 O3	C33 H26 N2 O3
Sum formula	C33 H26 N2 O3	C33 H26 N2 O3
Mr	498.56	498.56
Dx,g cm-3	1.326	1.326
Z	8	8
Mu (mm-1)	0.085	0.085
F000	2096.0	2096.0
F000'	2096.90	
h,k,lmax	22,10,36	22,10,36
Nref	8785[ 4485]	8093
Tmin,Tmax	0.985,0.988	0.633,0.745
Tmin'	0.919	

Correction method= # Reported T Limits: Tmin=0.633 Tmax=0.745  
AbsCorr = MULTI-SCAN

Data completeness= 1.80/0.92                      Theta(max)= 24.987

R(reflections)= 0.0455( 6207)                      wR2(reflections)= 0.1185( 8093)

S = 1.013                      Npar= 720

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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

STRVA01\_ALERT\_4\_C                      Flack test results are meaningless.  
From the CIF: \_refine\_ls\_abs\_structure\_Flack      0.300  
From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su      0.900

PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18) .....	6.20	Note
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	4.5	Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range	4.5	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range	4.6	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 2 H Uiso(max)/Uiso(min) Range	4.7	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C15 --C16A .	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C16A --C17 .	0.19	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C64	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00641	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.594	17	Report
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	84	%

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## ● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	4	Report
PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High .	0.900	Report
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size ....	1.00	mm
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	8%	Note
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 2 )	8%	Note
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C4 -C13 .	1.44	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C37 -C46 .	1.44	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C46 -C54	0.30	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C50 -C49B	0.29	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact O3B ..C61	2.95	Ang.
	x,y,z =	1_555	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	4	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	48%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT916_ALERT_2_G	Hooft y and Flack x Parameter Values Differ by .	0.16	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	4	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	11	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	1	Check

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

1 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
12 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
12 **ALERT type 3** Indicator that the structure quality may be low  
6 **ALERT type 4** Improvement, methodology, query or suggestion  
2 **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.

