

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) test5_a_pl

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: test5_a_pl

Bond precision:	C-C = 0.0040 A	Wavelength=0.71073	
Cell:	a=5.4660 (12)	b=10.025 (2)	c=15.193 (4)
	alpha=90	beta=90	gamma=90
Temperature:	146 K		
	Calculated	Reported	
Volume	832.5 (3)	832.5 (3)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C7 H11 N O4	C7 H11 N O4	
Sum formula	C7 H11 N O4	C7 H11 N O4	
Mr	173.17	173.17	
Dx, g cm ⁻³	1.382	1.382	
Z	4	4	
Mu (mm ⁻¹)	0.114	0.114	
F000	368.0	368.0	
F000'	368.23		
h, k, lmax	6, 11, 18	6, 11, 18	
Nref	1492 [899]	1488	
Tmin, Tmax	0.986, 0.989	0.359, 0.745	
Tmin'	0.942		

Correction method= # Reported T Limits: Tmin=0.359 Tmax=0.745
AbsCorr = NONE

Data completeness= 1.66/1.00 Theta(max)= 25.140

R(reflections)= 0.0419 (1317)	wR2(reflections)= 0.1026 (1488)
S = 1.079	Npar= 111

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 C

STRVA01_ALERT_4_C Flack test results are meaningless.
 From the CIF: _refine_ls_abs_structure_Flack -0.100
 From the CIF: _refine_ls_abs_structure_Flack_su 1.000
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.598 3 Report



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF Please Check
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.000 Report
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O2 . 109.4 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 1 Note
PLAT791_ALERT_4_G Model has Chirality at C3 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C5 (Sohnke SpGr) R Verify
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 66% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.20 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

- 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
14 **ALERT level G** = General information/check it is not something unexpected

- 2 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
4 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.

