

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_a

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: 1_a

Bond precision:	C-C = 0.0059 A	Wavelength=0.71073	
Cell:	a=21.9066 (15)	b=10.7688 (7)	c=13.5203 (9)
	alpha=90	beta=90	gamma=90
Temperature:	120 K		
	Calculated	Reported	
Volume	3189.5 (4)	3189.5 (4)	
Space group	P n a 21	P n a 21	
Hall group	P 2c -2n	P 2c -2n	
Moiety formula	C19 H18 O4	?	
Sum formula	C19 H18 O4	C4.75 H4.50 O	
Mr	310.33	77.58	
Dx, g cm ⁻³	1.293	1.293	
Z	8	32	
Mu (mm ⁻¹)	0.090	0.090	
F000	1312.0	1312.0	
F000'	1312.69		
h, k, lmax	28, 14, 17	28, 14, 17	
Nref	7423 [3868]	7306	
Tmin, Tmax	0.977, 0.982	0.549, 0.746	
Tmin'	0.977		

Correction method= # Reported T Limits: Tmin=0.549 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.89/0.98 Theta(max)= 27.636

R(reflections)= 0.0570 (5569)	wR2(reflections)=
S = 0.897	0.1640 (7306)
Npar= 419	

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.400
From the CIF: _refine_ls_abs_structure_Flack_su 0.800
PLAT230_ALERT_2_C Hirshfeld Test Diff for C9 --C12 . 6.8 s.u.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00594 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 14 Report



Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.800 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 11 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 3 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.40 Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **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
- 3 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
4 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.

