

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ta_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: ta_a

Bond precision:	C-C = 0.0020 A	Wavelength=1.54178	
Cell:	a=49.9332 (6)	b=49.9332 (6)	c=10.5479 (2)
	alpha=90	beta=90	gamma=120
Temperature:	173 K		
	Calculated	Reported	
Volume	22775.9 (7)	22775.9 (7)	
Space group	R -3	R -3	
Hall group	-R 3	-R 3	
Moiety formula	C56 H34 [+ solvent]	C56 H34, 2.5[CH3CH2CH2CH2CH3]	
Sum formula	C56 H34 [+ solvent]	C56 H34	
Mr	706.83	706.83	
Dx, g cm ⁻³	0.928	0.928	
Z	18	18	
Mu (mm ⁻¹)	0.400	0.400	
F000	6660.0	6660.0	
F000'	6677.41		
h, k, lmax	58, 58, 12	58, 58, 12	
Nref	8384	8379	
Tmin, Tmax	0.986, 0.992	0.660, 0.752	
Tmin'	0.961		

Correction method= # Reported T Limits: Tmin=0.660 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 63.892

R(reflections)= 0.0358 (6804)	wR2(reflections)=
S = 1.031	0.0940 (8379)
Npar= 505	

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

THETM01_ALERT_3_C The value of $\sin(\theta_{\max})/\lambda$ is less than 0.590
Calculated $\sin(\theta_{\max})/\lambda = 0.5824$
PLAT230_ALERT_2_C Hirshfeld Test Diff for C15 --C16 . 6.2 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C54 --C55 . 6.9 s.u.
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & Sth/L= 0.582 3 Report



Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C56 H34
Atom count from _chemical_formula_moiety: C68.5 H64
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.27 Why ?
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0001 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0001 Report
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 1 Note
PLAT909_ALERT_3_G Percentage of $I > 2\sigma(I)$ Data at $\theta(\text{Max})$ Still 58% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below $\theta(\text{Min})$. 1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 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
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
12 **ALERT level G** = General information/check it is not something unexpected

- 1 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
8 ALERT type 3 Indicator that the structure quality may be low
3 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.

