

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Cj1503

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: Cj1503

Bond precision: C-C = 0.0025 A Wavelength=1.54184

Cell: a=15.0415(2) b=10.7081(2) c=22.1277(2)
 alpha=90 beta=93.373(1) gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	3557.84(9)	3557.84(9)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C41 H60 N2	?
Sum formula	C41 H60 N2	C41 H60 N2
Mr	580.91	580.91
Dx,g cm-3	1.084	1.084
Z	4	4
Mu (mm-1)	0.458	0.458
F000	1280.0	1280.0
F000'	1283.03	
h,k,lmax	18,12,26	18,12,26
Nref	6607	6598
Tmin,Tmax	0.908,0.951	0.707,1.000
Tmin'	0.908	

Correction method= # Reported T Limits: Tmin=0.707 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 68.993

R(reflections)= 0.0559(5440) wR2(reflections)= 0.1563(6598)

S = 1.065 Npar= 395

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	4.0	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C38	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C39	Check	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		3.768	Check	
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).			10	Note	



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		1	Report	
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing		0.00020	Ang.	
PLAT153_ALERT_1_G	The s.u.'s on the Cell Axes are Equal ..(Note)			0.0002	Ang.	
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary				Please Do !	
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.0	Low	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			10	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
6 **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
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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.

Datablock Cj1503 - ellipsoid plot

