

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelxt_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: shelxt_a

Bond precision:	C-C = 0.0032 A	Wavelength=0.71075	
Cell:	a=3.9723(9)	b=13.700(3)	c=15.431(4)
	alpha=90	beta=91.128(6)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	839.6(3)	839.6(3)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C7 H6 N2 O5	C7 H6 N2 O5	
Sum formula	C7 H6 N2 O5	C7 H6 N2 O5	
Mr	198.14	198.14	
Dx, g cm-3	1.567	1.567	
Z	4	4	
Mu (mm-1)	0.136	0.136	
F000	408.0	408.0	
F000'	408.27		
h, k, lmax	5, 17, 20	5, 17, 20	
Nref	1922	1917	
Tmin, Tmax	0.968, 0.973	0.543, 1.000	
Tmin'	0.897		

Correction method= # Reported T Limits: Tmin=0.543 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 27.464

R(reflections)= 0.0604(1104) wR2(reflections)= 0.1400(1917)

S = 1.038 Npar= 166

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

PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N003	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	33.044	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	5.693	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.615	Check

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	10	Report
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..	0.80	mm
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	4	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	4	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	29%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact 0004 ..C00C	2.99	Ang.
	3/2-x, -1/2+y, 1/2-z =	2_645	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	23	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	84	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).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	4	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.1	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
17 **ALERT level G** = General information/check it is not something unexpected

- 3 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
7 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.

