

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	C-C = 0.0017 A	Wavelength=0.71073
Cell:	a=21.2110 (17)	b=3.7625 (3) c=13.9555 (11)
	alpha=90	beta=107.653 (3) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	1061.29 (15)	1061.29 (15)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C6 H5 N O2	?
Sum formula	C6 H5 N O2	C6 H5 N O2
Mr	123.11	123.11
Dx, g cm ⁻³	1.541	1.541
Z	8	8
Mu (mm ⁻¹)	0.118	0.118
F000	512.0	512.0
F000'	512.28	
h, k, lmax	34, 6, 23	34, 6, 22
Nref	2495	2478
Tmin, Tmax	0.972, 0.977	0.711, 0.747
Tmin'	0.965	

Correction method= # Reported T Limits: Tmin=0.711 Tmax=0.747
AbsCorr = PSI-SCANS

Data completeness= 0.993 Theta (max)= 35.905

R(reflections)= 0.0632 (1932)	wR2(reflections)= 0.1565 (2478)
S = 1.095	Npar= 107

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 psi-scans

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	0.69 eA-3
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	11.252 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.236 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3 Report



Alert level G

ABSTY01_ALERT_1_G Extra text has been found in the _exptl_absorpt_correction_type
field, which should be only a single keyword. A literature
citation should be included in the _exptl_absorpt_process_details
field.

PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4	Please Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	16 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2 Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please 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.	5 Info

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

- 4 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
2 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.

