

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) nai--xds-o6

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: nai--xds-o6

Bond precision: C-C = 0.0083 A

Wavelength=0.71073

Cell: a=7.6152(7) b=14.5507(17) c=21.281(2)
 alpha=104.024(9) beta=94.922(8) gamma=101.334(9)
Temperature: 293 K

	Calculated	Reported
Volume	2221.0(4)	2221.0(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C24 H14 Cl N3 O4), C H2 Cl2	C24 H14 Cl N3 O4, 0.5(C H2 Cl2)
Sum formula	C49 H30 Cl4 N6 O8	C24.50 H15 Cl2 N3 O4
Mr	972.59	486.29
Dx,g cm-3	1.454	1.454
Z	2	4
Mu (mm-1)	0.331	0.331
F000	996.0	996.0
F000'	997.60	
h,k,lmax	9,17,25	9,17,25
Nref	7825	7793
Tmin,Tmax	0.902,0.933	0.807,1.000
Tmin'	0.899	

Correction method= # Reported T Limits: Tmin=0.807 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 25.023

R(reflections)= 0.0864(3862)

wR2(reflections)= 0.2842(7793)

S = 1.049

Npar= 607

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

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.28	Report
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C018	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C1	0.170	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00831	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	14.623	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.412	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	30	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1	Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S .	23.26	Check



Alert level G

PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ		Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.15	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C102 ..C00K	3.23	Ang.
	2-x,1-y,1-z =	2_766	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	92	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	5	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.8	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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

- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
2 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.

