

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) xln24_0m

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: xln24_0m

Bond precision:	C-C = 0.0094 Å	Wavelength=1.54178
Cell:	a=19.4803(13)	b=14.8269(10) c=21.4352(15)
	alpha=90	beta=90.484(2) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	6191.0(7)	6191.0(7)
Space group	C c	C 1 c 1
Hall group	C -2yc	C -2yc
Moiety formula	C51 F51 O8 P2 Yb, C H2 Cl2	C51 F51 O8 P2 Yb, C H2 Cl2
Sum formula	C52 H2 Cl2 F51 O8 P2 Yb	C52 H2 Cl2 F51 O8 P2 Yb
Mr	2029.42	2029.42
Dx,g cm-3	2.177	2.177
Z	4	4
Mu (mm-1)	6.057	6.057
F000	3884.0	3884.0
F000'	3880.34	
h,k,lmax	24,18,26	23,18,26
Nref	12225[6117]	10675
Tmin,Tmax	0.169,0.298	0.084,1.000
Tmin'	0.059	

Correction method= # Reported T Limits: Tmin=0.084 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.75/0.87 Theta(max)= 72.367

R(reflections)= 0.0310(10635) wR2(reflections)= 0.0829(10675)

S = 1.076 Npar= 1074

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 B

PLAT090_ALERT_3_B	Poor Data / Parameter Ratio (Zmax > 18)	5.65	Note
PLAT213_ALERT_2_B	Atom C47 has ADP max/min Ratio	4.1	prolat
PLAT987_ALERT_1_B	The Flack x is >> 0 - Do a BASF/TWIN Refinement		Please Check

Alert level C

PLAT213_ALERT_2_C	Atom F18 has ADP max/min Ratio	3.7	prolat
PLAT213_ALERT_2_C	Atom F19 has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom F28 has ADP max/min Ratio	3.2	oblate
PLAT213_ALERT_2_C	Atom F29 has ADP max/min Ratio	3.1	prolat
PLAT213_ALERT_2_C	Atom F46 has ADP max/min Ratio	3.8	prolat
PLAT213_ALERT_2_C	Atom F47 has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom F48 has ADP max/min Ratio	3.7	prolat
PLAT213_ALERT_2_C	Atom F49B has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom F50B has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C	Atom C22 has ADP max/min Ratio	3.3	prolat
PLAT213_ALERT_2_C	Atom C23 has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C34 has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C	Atom C51 has ADP max/min Ratio	3.6	oblate
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) Range	3.9	Ratio
PLAT220_ALERT_2_C	Large Non-Solvent F Ueq(max)/Ueq(min) Range	4.8	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C22 -- C23 ..	0.17	Ang.
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for		C51 Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0094	Ang.
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600		3 Report

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	7	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	17.49	Why ?
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT242_ALERT_2_G	Low Ueq as Compared to Neighbors for	C46	Check
PLAT242_ALERT_2_G	Low Ueq as Compared to Neighbors for	C47	Check
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =	3 Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact F3 .. C21 ..	2.87	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F32 .. C15 ..	2.91	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F34 .. C8 ..	2.93	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F43 .. C27 ..	2.90	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F43 .. C26 ..	2.93	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact C12 .. F49A ..	3.08	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F2 .. F50B ..	2.82	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F4 .. F29 ..	2.83	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F6 .. F34 ..	2.78	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F7 .. F51A ..	2.80	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F7 .. F51B ..	2.82	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F12 .. F24 ..	2.78	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F12 .. F32 ..	2.81	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F13 .. F18 ..	2.64	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F14 .. F36 ..	2.76	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F19 .. F51B ..	2.60	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F19 .. F42 ..	2.79	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F33 .. F50B ..	2.80	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F38 .. F51A ..	2.61	Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	74	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	50	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check

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

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

