

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) r20231108c

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: r20231108c

Bond precision:	C-C = 0.0082 A	Wavelength=0.71073
Cell:	a=12.74654 (17)	b=14.6333 (2) c=12.86588 (19)
	alpha=90	beta=97.5620 (13) gamma=90
Temperature:	113 K	
	Calculated	Reported
Volume	2378.92 (6)	2378.93 (6)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C14 H15 Cl	1 (C14 H15 Cl)
Sum formula	C14 H15 Cl	C14 H15 Cl
Mr	218.71	218.71
Dx, g cm ⁻³	1.221	1.221
Z	8	8
Mu (mm ⁻¹)	0.285	0.285
F000	928.0	928.0
F000'	929.47	
h, k, lmax	16, 19, 17	16, 19, 17
Nref	11770 [6111]	11769
Tmin, Tmax	0.921, 0.950	0.555, 1.000
Tmin'	0.902	

Correction method= # Reported T Limits: Tmin=0.555 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.93/1.00 Theta(max)= 28.282

R(reflections)= 0.0929 (11051)	wR2(reflections)=
S = 1.119	0.2444 (11769)
Npar= 748	

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.57	Report
PLAT213_ALERT_2_C	Atom ClA has ADP max/min Ratio	3.1	prolat
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C43 --C44 .	5.5	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C1 --C2 .	0.23	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C27 --C28 .	0.16	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C30 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0082	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.984	Check
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	66	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	60	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.15	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	24	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for Cl2 --C26 .	7.2	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	100%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 2)	100%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 5)	100%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 6)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 1)	18.66	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	22.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 5)	11.34	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 6)	7.50	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	421	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	3	Note
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	3	Check

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
11 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

