

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) t

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: t

Bond precision: C-C = 0.0127 Å Wavelength=1.54178

Cell: a=9.8911(4) b=15.4147(6) c=15.4438(7)
 alpha=87.166(2) beta=80.070(3) gamma=86.647(3)
Temperature: 173 K

	Calculated	Reported
Volume	2313.59(17)	2313.59(17)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C26 H18 Cl N3 O [+ solvent]	C26 H18 Cl N3 O [+ solvent]
Sum formula	C26 H18 Cl N3 O [+ solvent]	C26 H18 Cl N3 O
Mr	423.88	423.88
Dx, g cm ⁻³	1.217	1.217
Z	4	4
Mu (mm ⁻¹)	1.627	1.627
F000	880.0	880.0
F000'	883.77	
h, k, lmax	11, 17, 17	11, 17, 17
Nref	15228[7614]	14698
Tmin, Tmax	0.783, 0.823	0.678, 0.753
Tmin'	0.783	

Correction method= # Reported T Limits: Tmin=0.678 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.93/0.97 Theta(max)= 63.657

R(reflections)= 0.0665(8767)	wR2(reflections)=
S = 0.940	0.1856(14698)
Npar= 1121	

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

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01274 Ang.



Alert level C

THETM01_ALERT_3_C The value of $\sin(\theta_{\max})/\text{wavelength}$ is less than 0.590
Calculated $\sin(\theta_{\max})/\text{wavelength} = 0.5812$
PLAT089_ALERT_3_C Poor Data / Parameter Ratio ($Z_{\max} < 18$) 6.79 Note
PLAT213_ALERT_2_C Atom Cl2 has ADP max/min Ratio 4.0 prolat
PLAT213_ALERT_2_C Atom C30 has ADP max/min Ratio 3.4 prolat
PLAT213_ALERT_2_C Atom C31 has ADP max/min Ratio 3.2 prolat
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of N5 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C30 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C57 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C29 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C31 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C56 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.6 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.2 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.581 4 Report
PLAT987_ALERT_1_C The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check



Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 11 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.057 Note
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 6 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report
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PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report
PLAT432_ALERT_2_G Short Inter X...Y Contact O1 ..C43 . 2.95 Ang.
1+x,y,z = 1_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O2 ..C68 . 2.87 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O2 ..C69 . 3.00 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O3 ..C94 . 2.89 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O3 ..C95 . 2.96 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O4 ..C17 . 2.92 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O4 ..C19 . 2.98 Ang.
x,y,z = 1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl1 ..C12 . 3.35 Ang.
1+x,y,-1+z = 1_654 Check

PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	9	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

2	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
21	ALERT type 2	Indicator that the structure model may be wrong or deficient
11	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

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.

