

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: alectinib_hydrochloride

Bond precision: C-C = 0.0055 A Wavelength=1.54449

Cell: a=20.3873(10) b=10.4505(4) c=12.6827(5)
 alpha=90 beta=93.105(2) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	2698.2(2)	2698.177(6)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C30 H35 N4 O2, Cl	C30 H35 N4 O2 +, Cl -
Sum formula	C30 H35 Cl N4 O2	C30 H35 Cl N4 O2
Mr	519.07	519.07
Dx, g cm ⁻³	1.278	1.278
Z	4	4
Mu (mm ⁻¹)	1.521	1.521
F000	1104.0	1104.0
F000'	1108.34	
h, k, lmax	18, 9, 11	
Nref	2174	
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.000 Theta (max) =

R(reflections)= wR2(reflections)=
S = Npar=

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

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	O2	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N1	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N3	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N4	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C8	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C28	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C29	Check
PLAT340_ALERT_3_C	Low	Bond Precision on	C-C Bonds	0.00552	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C2 - H2	1.11	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C4 - H4A	1.12	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C18 - H18A	1.13	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C18 - H18B	1.12	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C19 - H19A	1.12	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C20 - H20B	1.11	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C24 - H24	1.11	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C26 - H26A	1.13	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C26 - H26B	1.11	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C27 - H27A	1.16	Ang.
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C28 - H28B	1.15	Ang.
PLAT353_ALERT_3_C	Long	N-H (N0.87,N1.01A)	N1 - H1	1.04	Ang.
PLAT361_ALERT_2_C	Long	C(sp3)-C(sp3) Bond	C25 - C26	1.65	Ang.
PLAT702_ALERT_1_C	Angle	Calc 108.9(6), Rep 109.8(5), Dev..		1.50	Sigma
	C30	-C29	-H29B	1_555	1_555 1_555 # 137 Check

Alert level G

RADNT01_ALERT_1_G Extra text has been found in the _diffrn_radiation_type field.

Radiation given as Cu K\alpha~1~, K\alpha~2~

Radiation identified as Cu K\alpha~1~

PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	194	Units
PLAT158_ALERT_4_G	The Input Unitcell is NOT Standard/Reduced	Please	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C23	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C24	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C25	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C26	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	105	Note
PLAT982_ALERT_1_G	The C-f' = 0.0033 Deviates from IT-value =	0.0181	Check
PLAT982_ALERT_1_G	The Cl-f' = 0.1484 Deviates from IT-value =	0.3639	Check
PLAT982_ALERT_1_G	The N-f' = 0.0061 Deviates from IT-value =	0.0311	Check
PLAT982_ALERT_1_G	The O-f' = 0.0106 Deviates from IT-value =	0.0492	Check
PLAT983_ALERT_1_G	The C-f" = 0.0016 Deviates from IT-Value =	0.0091	Check
PLAT983_ALERT_1_G	The Cl-f" = 0.1585 Deviates from IT-Value =	0.7018	Check
PLAT983_ALERT_1_G	The N-f" = 0.0033 Deviates from IT-Value =	0.0180	Check
PLAT983_ALERT_1_G	The O-f" = 0.0060 Deviates from IT-Value =	0.0322	Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

22 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

16 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
14 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

PLATON version of 13/12/2023; check.def file version of 13/12/2023

